

=> d his ful

(FILE 'HOME' ENTERED AT 16:50:24 ON 13 MAR 2006)

FILE 'REGISTRY' ENTERED AT 16:51:22 ON 13 MAR 2006

L5 STR  
L7 118852 SEA SSS FUL L5  
L8 STR  
L9 157 SEA SUB=L7 SSS FUL L8  
L10 STR  
L11 18 SEA SUB=L9 SSS FUL L10

FILE 'HCAPLUS' ENTERED AT 16:55:16 ON 13 MAR 2006

L12 7 SEA ABB=ON PLU=ON L11  
D STAT QUE  
D IBIB ABS HITSTR L12 1-7

FILE 'REGISTRY' ENTERED AT 16:56:25 ON 13 MAR 2006

D IDE CAN L11 1-18

FILE 'BEILSTEIN' ENTERED AT 17:02:58 ON 13 MAR 2006

L13 4 SEA SSS FUL L10  
L14 3 SEA ABB=ON PLU=ON L13 NOT L11  
D STAT QUE L14  
D BRN CN MF FW STR PHARM RX L14 1-3

FILE 'HCAPLUS' ENTERED AT 17:37:44 ON 13 MAR 2006

L15 43 SEA ABB=ON PLU=ON ("EMIG P"/AU OR "EMIG PETER"/AU)  
L16 41 SEA ABB=ON PLU=ON L15 NOT L12  
D STAT QUE L16  
D IBIB ABS L16 1-41  
L17 67 SEA ABB=ON PLU=ON ("GUNTHER E"/AU OR "GUNTHER ECKHARD"/AU)  
NOT (L12 OR L16)  
D STAT QUE L17  
D IBIB ABS L17 1-67  
L18 1 SEA ABB=ON PLU=ON (("AUE B J"/AU OR "AUE BEATE"/AU)) NOT  
(L12 OR L16 OR L17)  
D STAT QUE NOS L18  
D IBIB ABS L18 1  
L19 41 SEA ABB=ON PLU=ON (("POLYMEROPOULOS E"/AU OR "POLYMEROPOULOS  
E E"/AU OR "POLYMEROPOULOS EMANUELE E"/AU OR "POLYMEROPOULOS  
EMMANUEL"/AU OR "POLYMEROPOULOS EMMANUEL E"/AU)) NOT (L12 OR  
L16 OR L17 OR L18)  
D STAT QUE L19 NOS  
D IBIB ABS L19 1-41  
L20 12 SEA ABB=ON PLU=ON (("BAASNER S"/AU OR "BAASNER SIIKE"/AU OR  
"BAASNER SILKE"/AU)) NOT (L12 OR L16 OR L17 OR L18 OR L19)  
D STAT QUE L20 NOS  
D IBIB ABS L20 1-12  
L21 1218 SEA ABB=ON PLU=ON ("SCHMIDT P"/AU OR "SCHMIDT P A"/AU OR  
"SCHMIDT P B JR"/AU OR "SCHMIDT P C"/AU OR "SCHMIDT P D"/AU OR  
"SCHMIDT P E"/AU OR "SCHMIDT P F"/AU OR "SCHMIDT P G"/AU OR  
"SCHMIDT P H"/AU OR "SCHMIDT P HENRY"/AU OR "SCHMIDT P J"/AU  
OR "SCHMIDT P K"/AU OR "SCHMIDT P K H"/AU OR "SCHMIDT P KARL  
HEINZ"/AU OR "SCHMIDT P L"/AU OR "SCHMIDT P M"/AU OR "SCHMIDT  
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P JR"/AU OR "SCHMIDT P R"/AU OR "SCHMIDT P R L"/AU OR "SCHMIDT  
P S"/AU OR "SCHMIDT P T"/AU OR "SCHMIDT P U"/AU OR "SCHMIDT P  
V"/AU OR "SCHMIDT P W"/AU OR "SCHMIDT P WORSE"/AU OR "SCHMIDT  
P WORSOE"/AU) OR SCHMIDT PETER ?/AU

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Ward 10\_651590 - - History

FILE 'HCAPLUS' ENTERED AT 17:45:08 ON 13 MAR 2006

L22 100932 SEA ABB=ON PLU=ON L7  
L23 5 SEA ABB=ON PLU=ON (L21 AND L22) NOT (L12 OR L16 OR L17 OR  
L18 OR L19 OR L20)  
D STAT QUE  
D IBIB ABS HITSTR L23 1-5

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 12 MAR 2006 HIGHEST RN 876514-29-3

DICTIONARY FILE UPDATES: 12 MAR 2006 HIGHEST RN 876514-29-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

Structure search iteration limits have been increased. See HELP SLIMITS  
for details.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

FILE HCAPLUS

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FILE COVERS 1907 - 13 Mar 2006 VOL 144 ISS 12

FILE LAST UPDATED: 12 Mar 2006 (20060312/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE BEILSTEIN

FILE LAST UPDATED ON JANUARY 17, 2006

FILE COVERS 1771 TO 2005.

FILE CONTAINS 9,428,406 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

\*\*\*\*\*  
\* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. \*  
\* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE \*  
\* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE \*  
\* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. \*  
\* FOR PRICE INFORMATION SEE HELP COST \*  
\*\*\*\*\*

NEW

\* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.  
\* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.

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FILE 'HCAPLUS' ENTERED AT 16:55:16 ON 13 MAR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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```

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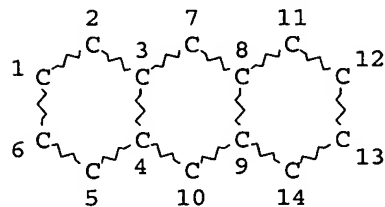
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FILE COVERS 1907 - 13 Mar 2006 VOL 144 ISS 12
FILE LAST UPDATED: 12 Mar 2006 (20060312/ED)
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New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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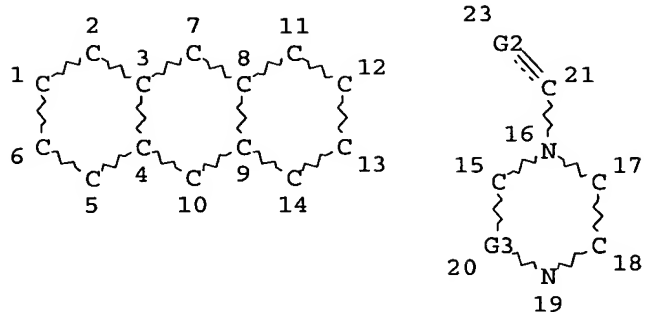
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=> d stat que
L5 STR
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DEFAULT ECLEVEL IS LIMITED
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GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 14
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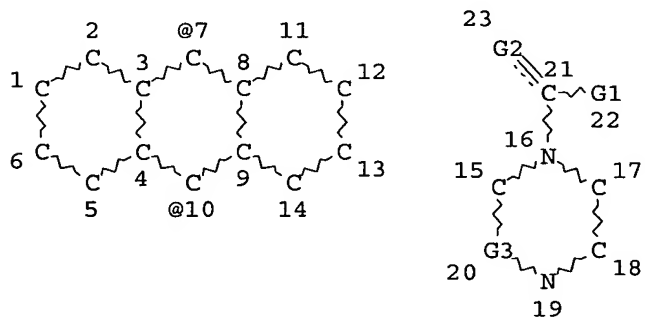
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L7 118852 SEA FILE=REGISTRY SSS FUL L5
L8 STR
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GRAPH ATTRIBUTES:  
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 NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE  
 L9 157 SEA FILE=REGISTRY SUB=L7 SSS FUL L8  
 L10 STR



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GRAPH ATTRIBUTES:  
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STEREO ATTRIBUTES: NONE  
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 L12 7 SEA FILE=HCAPLUS ABB=ON PLU=ON L11

=>  
 =>

=> d ibib abs hitstr l12 1-7

L12 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:53490 HCAPLUS

DOCUMENT NUMBER: 142:309180

TITLE: Design and synthesis of a focused library of novel aryl- and heteroaryl-ketopiperazides

AUTHOR(S): Gerlach, Matthias; Claus, Eckhard; Baasner, Siike; Mueller, Gilbert; Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel, Juergen

CORPORATE SOURCE: Drug Discovery, Zentaris GmbH, Frankfurt am Main, Germany

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (2004), 337(12), 695-703

CODEN: ARPMAS; ISSN: 0365-6233

PUBLISHER: Wiley-VCH Verlag GmbH &amp; Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

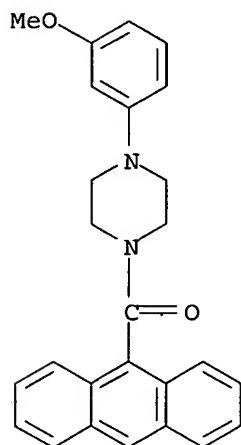
AB 1-Phenyl-4-piperazinyl-carbonyl-substituted nitrogen-containing heterocycles were discovered at Zentaris as a new class of potent, synthetic, small mol. tubulin inhibitors with strong antiproliferative activity. The lead structure of this class, D-24203, proved to be a potent inhibitor of in vivo tumor growth in different xenograft models including mammary and renal cancers. As part of our efforts in the lead optimization process to expand structural diversity as well as to optimize bioavailability parameters such as solubility and metabolic stability for these compds., we produced and evaluated a focused library containing 320 compds. Five new heterocyclic compound classes with comparable activity properties in the cytotoxicity and tubulin polymerization assay could be identified. In silico calculated bioavailability parameters for selected library members provides new compound classes with improved solubility properties. Library design, development of adequate solution phase methodol., and synthesis will be presented, as well as results of lead optimization.

IT 848084-63-9 848084-64-0

RL: PAC (Pharmacological activity); BIOL (Biological study)  
(design and synthesis of a focused library of novel aryl- and heteroaryl-ketopiperazides)

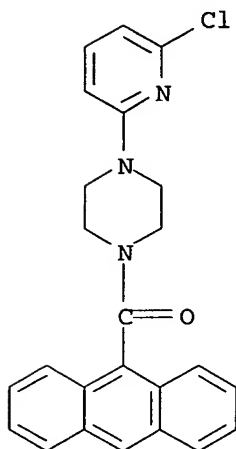
RN 848084-63-9 HCAPLUS

CN Piperazine, 1-(9-anthracenylcarbonyl)-4-(3-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 848084-64-0 HCAPLUS

CN Piperazine, 1-(9-anthracenylcarbonyl)-4-(6-chloro-2-pyridinyl)- (9CI) (CA  
INDEX NAME)



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:75996 HCAPLUS

DOCUMENT NUMBER: 140:146164

TITLE: Preparation of (anthracenyl)(piperazinyl)methanones as  
antitumor agents

INVENTOR(S): Emig, Peter; Guenther, Eckhard; Aue, Beate;  
Polymeropoulos, Emmanuel; Baasner, Silke; Schmidt,  
Peter

PATENT ASSIGNEE(S): Zentaris A.-G., Germany

SOURCE: Ger. Offen., 31 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

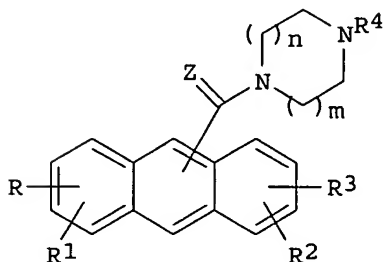
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10232525	A1	20040129	DE 2002-10232525	20020718
PRIORITY APPLN. INFO.:			DE 2002-10232525	20020718
OTHER SOURCE(S):	MARPAT	140:146164		

GI



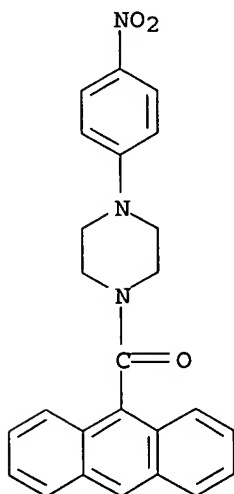
I

AB Title compds. [I; R-R3 = H, OH, halo, (branched) alkyl, cycloalkyl, alkylcarbonyl, alkoxy, arylalkoxy, etc.; Z = O, S; n, m = 0-4; R4 = (branched) (saturated) (substituted) alkyl, aryl, arylalkyl, etc.], were prepared Thus, anthracene-9-carboxylic acid in DMF was treated successively with N-methylmorpholine, 1-(4-nitrophenyl)piperazine, and Py-BOP followed by stirring for 4 h at room temperature to give 79.7% 1-(4-nitrophenyl)-4-(anthracen-9-ylcarbonyl)piperazine. Anthracen-9-yl-[4-(3,5-dimethoxyphenyl)piperazin-1-yl]methanone inhibited proliferation of different human tumor cells in XTT cytotoxicity test with EC50 = 0.047->3.16 µg/mL.

IT 647854-29-3P 647854-30-6P 647854-31-7P  
 647854-32-8P 647854-33-9P 647854-34-0P  
 647854-35-1P 647854-36-2P 647854-37-3P  
 647854-38-4P 647854-39-5P 647854-40-8P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of (anthracenyl)(piperazinyl)methanones as antitumor agents)

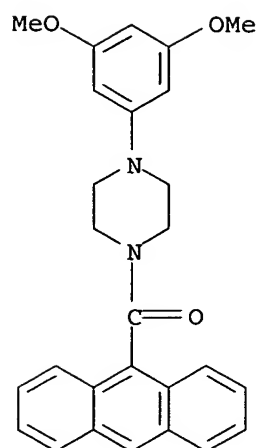
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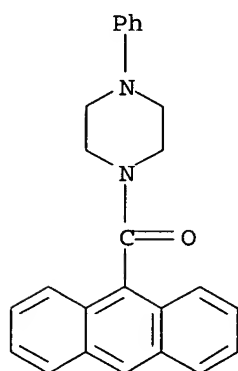


RN 647854-30-6 HCAPLUS

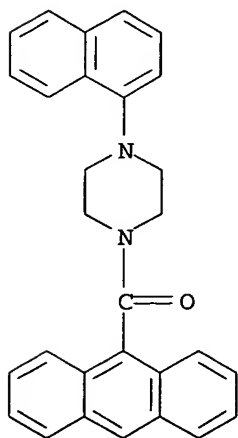
CN Piperazine, 1-(9-anthracenylcarbonyl)-4-(3,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



RN 647854-31-7 HCAPLUS  
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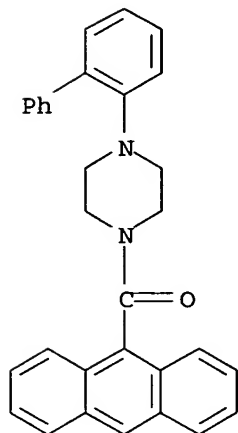


RN 647854-32-8 HCAPLUS  
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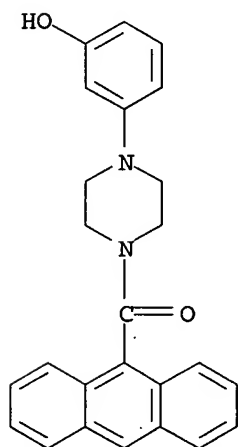




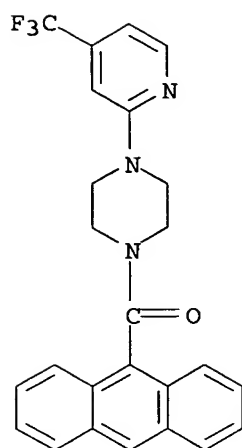
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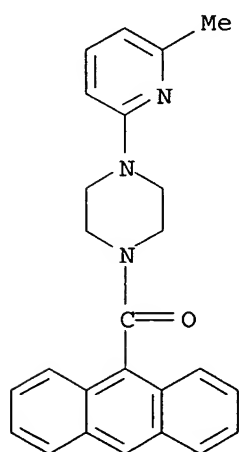
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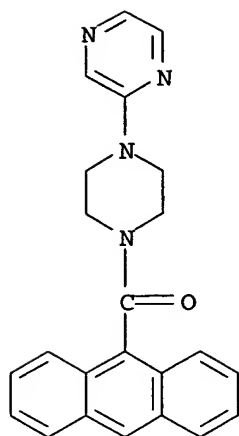
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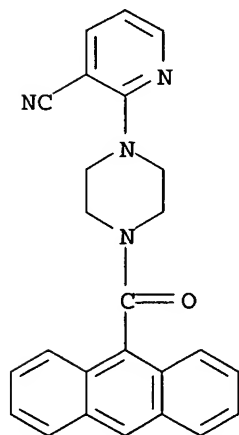
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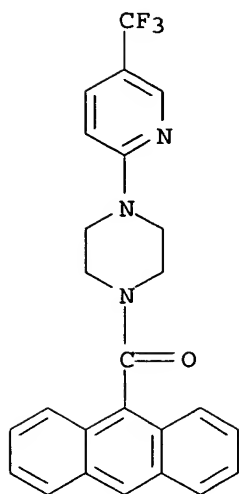
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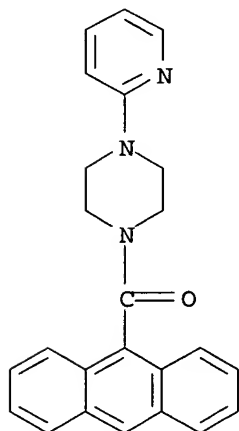
RN 647854-38-4 HCAPLUS  
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RN 647854-39-5 HCAPLUS  
 CN Piperazine, 1-(9-anthracenylcarbonyl)-4-[5-(trifluoromethyl)-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 647854-40-8 HCAPLUS  
 CN Piperazine, 1-(9-anthracenylcarbonyl)-4-(2-pyridinyl)- (9CI) (CA INDEX NAME)



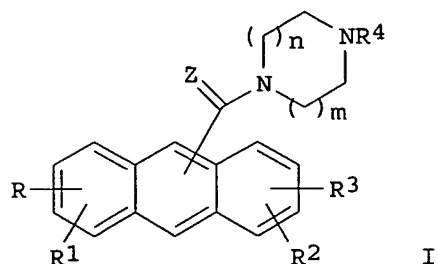
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2004:60486 HCAPLUS  
 DOCUMENT NUMBER: 140:111430  
 TITLE: Preparation of (anthracenyl)(piperazinyl)methanones as antitumor agents  
 INVENTOR(S): Emig, Peter; Guenther, Eckhard; Aue, Beate; Polymeropoulos, Emmanuel; Baasner, Silke; Schmidt, Peter  
 PATENT ASSIGNEE(S): Zentaris GmbH, Germany  
 SOURCE: PCT Int. Appl., 70 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004007470	A1	20040122	WO 2003-EP5156	20030516
W: AU, BR, BY, CA, CN, CO, GE, HR, HU, ID, IL, IN, IS, JP, KR, KZ, LT, LV, MK, MX, NO, NZ, PH, PL, RO, RU, SG, UA, UZ, YU, ZA				
RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
AU 2003232785	A1	20040202	AU 2003-232785	20030516
EP 1521748	A1	20050413	EP 2003-763626	20030516
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, TR, BG, CZ, EE, HU, SK				
CN 1668604	A	20050914	CN 2003-816919	20030516
JP 2005537258	T2	20051208	JP 2004-520367	20030516
CA 2435399	AA	20040117	CA 2003-2435399	20030717
US 2004110756	A1	20040610	US 2003-621590	20030717
PRIORITY APPLN. INFO.:			US 2002-396683P	P 20020717
			WO 2003-EP5156	W 20030516

OTHER SOURCE(S): MARPAT 140:111430  
GI



AB Title compds. [I; R-R3 = H, OH, halo, (branched) alkyl, cycloalkyl, alkylcarbonyl, alkoxy, arylalkoxy, etc.; Z = O, S; n, m = 0-4; R4 = (branched) (saturated) (substituted) alkyl, aryl, arylalkyl, etc.], were prepared Thus, anthracene-9-carboxylic acid in DMF was treated successively with N-methylmorpholine, 1-(4-nitrophenyl)piperazine, and Py-BOP followed by stirring for 4 h at room temperature to give 79.7% 1-(4-nitrophenyl)-4-(anthracen-9-ylcarbonyl)piperazine. Anthracen-9-yl-[4-(3,5-dimethoxyphenyl)piperazin-1-yl]methanone inhibited proliferation of different human tumor cells in XTT cytotoxicity test with EC50 = 0.047->3.16 µg/mL.

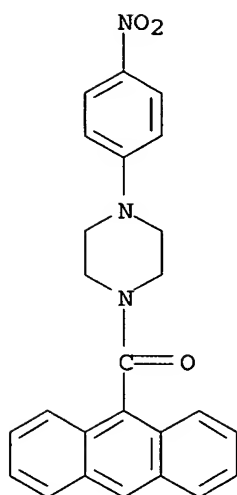
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647854-32-8P 647854-33-9P 647854-34-0P  
647854-35-1P 647854-36-2P 647854-37-3P  
647854-38-4P 647854-39-5P 647854-40-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

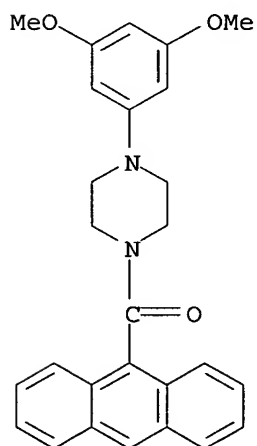
(preparation of (anthracenyl)(piperazinyl)methanones as antitumor agents)

RN 647854-29-3 HCAPLUS

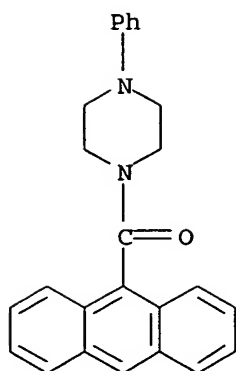
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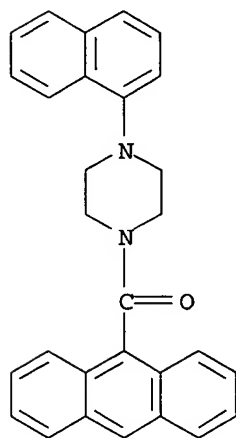
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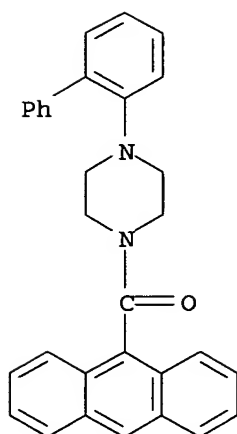
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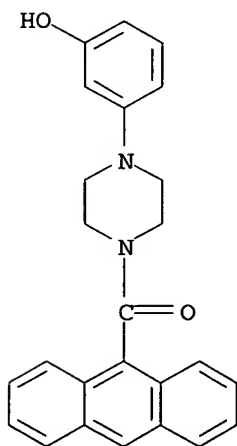
RN 647854-32-8 HCAPLUS  
 CN Piperazine, 1-(9-anthracenylcarbonyl)-4-(1-naphthalenyl)- (9CI) (CA INDEX NAME)



RN 647854-33-9 HCAPLUS  
 CN Piperazine, 1-(9-anthracenylcarbonyl)-4-[1,1'-biphenyl]-2-yl- (9CI) (CA INDEX NAME)

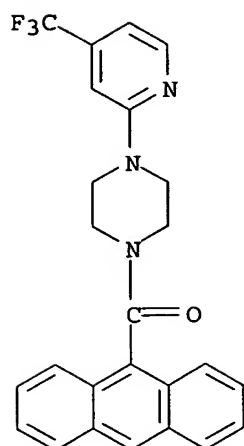


RN 647854-34-0 HCAPLUS  
 CN Piperazine, 1-(9-anthracenylcarbonyl)-4-(3-hydroxyphenyl)- (9CI) (CA  
 INDEX NAME)

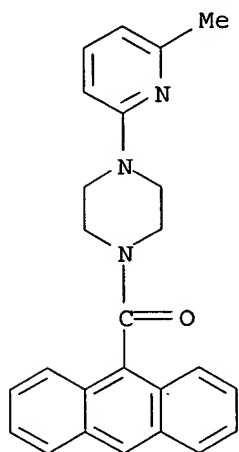


RN 647854-35-1 HCAPLUS  
 CN Piperazine, 1-(9-anthracenylcarbonyl)-4-[4-(trifluoromethyl)-2-pyridinyl]-  
 (9CI) (CA INDEX NAME)

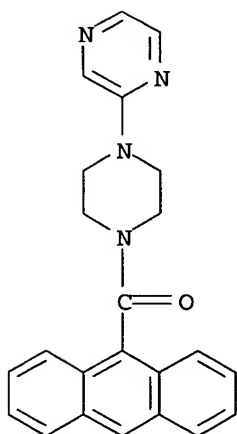




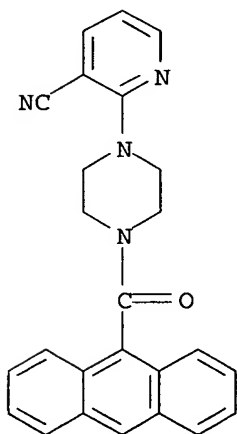
RN 647854-36-2 HCAPLUS  
 CN Piperazine, 1-(9-anthracenylcarbonyl)-4-(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)



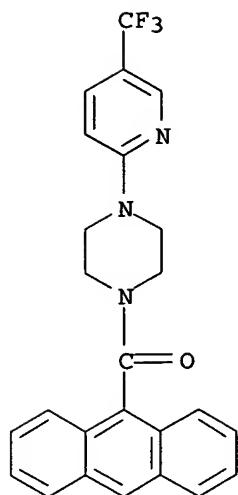
RN 647854-37-3 HCAPLUS  
 CN Piperazine, 1-(9-anthracenylcarbonyl)-4-pyrazinyl- (9CI) (CA INDEX NAME)



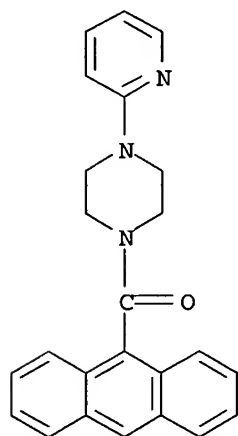
RN 647854-38-4 HCAPLUS  
 CN Piperazine, 1-(9-anthracenylcarbonyl)-4-(3-cyano-2-pyridinyl)- (9CI) (CA INDEX NAME)



RN 647854-39-5 HCAPLUS  
 CN Piperazine, 1-(9-anthracenylcarbonyl)-4-[5-(trifluoromethyl)-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 647854-40-8 HCAPLUS  
 CN Piperazine, 1-(9-anthracenylcarbonyl)-4-(2-pyridinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:696782 HCAPLUS

DOCUMENT NUMBER: 139:230625

TITLE: Preparation of bipiperidinyll and related compounds as acetyl CoA carboxylase inhibitors useful against metabolic syndrome and other disorders

INVENTOR(S): Perry, David Austen; Harwood, Harold James, Jr.

PATENT ASSIGNEE(S): Pfizer Products Inc., USA

SOURCE: PCT Int. Appl., 181 pp.

CODEN: PIXXD2

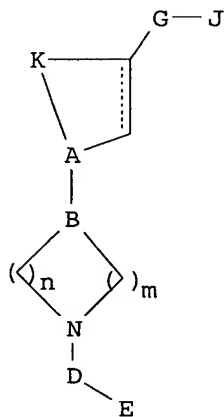
DOCUMENT TYPE: Patent

LANGUAGE: English

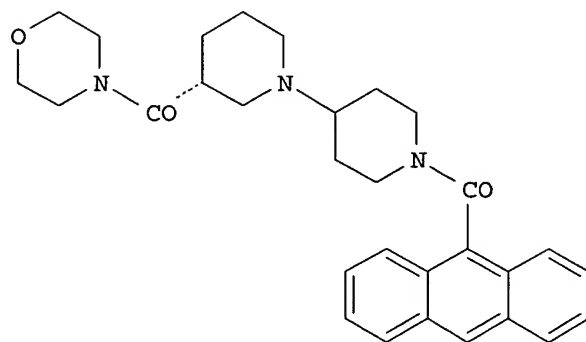
FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003072197	A1	20030904	WO 2003-IB573	20030217
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003248354	A1	20030909	AU 2003-248354	20030217
EP 1478437	A1	20041124	EP 2003-742882	20030217
EP 1478437	B1	20050831		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AT 303178	E	20050915	AT 2003-742882	20030217
US 2003187254	A1	20031002	US 2003-370844	20030220
US 6979741	B2	20051227		
NO 2004004034	A	20041124	NO 2004-4034	20040924
PRIORITY APPLN. INFO.:			US 2002-365358P	P 20020227
			WO 2003-IB573	W 20030217
OTHER SOURCE(S):	MARPAT 139:230625			
GI				



I



II

AB Acetyl CoA carboxylase (ACC) inhibitors (shown as I; variables defined below; most examples include the bipiperidiny ring system, e.g. (anthracen-9-yl) [(3R)-3-(morpholine-4-carbonyl) [1,4']bipiperidiny-1'-yl]methanone), pharmaceutical compns. containing such compds. and the use of such compds. to treat for example, Metabolic Syndrome, atherosclerosis, diabetes and obesity are disclosed. None of pharmacol. activity, therapeutic uses and methods of preparation is claimed and pharmacol. data are not included. More than 200 example preps. and/or characterization data are included for I and intermediates. For I: A-B is N-CH or CH-N; K is (CH<sub>2</sub>)<sub>r</sub> (r = 2-4); m and n = 1-3 when A-B is N-CH or 2 or 3 when A-B is CH-N; the dashed line = the presence of an optional double bond; D is carbonyl or sulfonyl. E is either (a) a bicyclic ring consisting of two

fused fully unsatd. 5-7 membered rings, taken independently, each of said rings optionally having 1-4 heteroatoms = O, S and N; or (b) a tricyclic ring consisting of two fused fully unsatd. 5-7 membered rings, taken independently, each of said rings optionally having 1-4 heteroatoms = O, S and N, said two fused rings fused to a 3rd partially saturated, fully unsatd. or fully saturated 5-7 membered ring, said 3rd ring optionally having 1-4 heteroatoms = O, S and N. Or (c) a tetracyclic ring comprising a bicyclic ring consisting of two fused fully unsatd. 5-7 membered rings, taken independently, each of said rings optionally having 1-4 heteroatoms = O, S and N, said bicyclic ring fused to two fully saturated, partially saturated or fully unsatd. 5-7 membered monocyclic rings taken independently, each of said rings optionally having 1-4 heteroatoms = O, S and N or said bicyclic ring fused to a 2nd bicyclic ring consisting of two fused fully saturated, partially saturated or fully unsatd. 5-7 membered rings, taken independently, each of said rings optionally having 1-4 heteroatoms = O, S and N; or (d) a teraryl ring comprising a fully unsatd. 5-7 membered ring, said ring optionally having 1-4 heteroatoms = O, S and N, and said ring disubstituted independently with a fully unsatd. 5-7 membered ring to form a teraryl nonfused ring system, each of said substituent rings optionally having 1-4 heteroatoms = O, S and N. G is carbonyl, sulfonyl or CR7R8 (R7 and R8 = H, (C1-C6)alkyl, (C2-C6) alkenyl or (C2-C6)alkynyl or a 5-7 membered partially saturated, fully saturated or fully unsatd. ring optionally having one heteroatom = O, S and N); J is OR1, NR2R3 or CR4R5R6; addnl. details including provisos are given in the claims.

IT 591781-15-6P, (Anthracen-9-yl) [4-[(1R,3R)-3-[(morpholin-4-yl)carbonyl]cyclohexyl]piperazin-1-yl]methanone 591781-16-7P, (Anthracen-9-yl) [4-[(1S,3R)-3-[(morpholin-4-yl)carbonyl]cyclohexyl]piperazin-1-yl]methanone

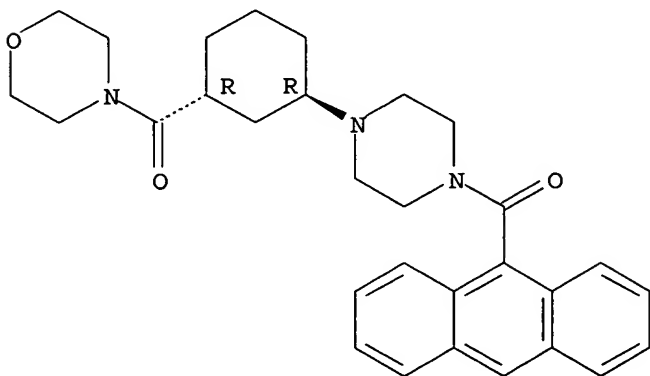
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of bipiperidinyl and related compds. as acetyl CoA carboxylase inhibitors useful against metabolic syndrome and other disorders)

RN 591781-15-6 HCAPLUS

CN Morpholine, 4-[[[(1R,3R)-3-[4-(9-anthracenylcarbonyl)-1-piperazinyl]cyclohexyl]carbonyl]- (9CI) (CA INDEX NAME)

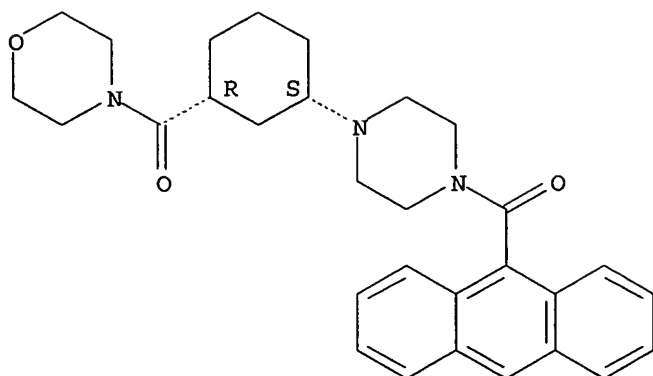
Absolute stereochemistry.



RN 591781-16-7 HCAPLUS

CN Morpholine, 4-[[[(1R,3S)-3-[4-(9-anthracenylcarbonyl)-1-piperazinyl]cyclohexyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:641466 HCAPLUS

DOCUMENT NUMBER: 133:350193

TITLE: Non-amide-based combinatorial libraries derived from N-BOC-iminodiacetic acid: solution-phase synthesis of piperazinone libraries with activity against LEF-1/ $\beta$ -catenin-mediated transcription

AUTHOR(S): Boger, Dale L.; Goldberg, Joel; Satoh, Shigeki; Ambroise, Yves; Cohen, Steven B.; Vogt, Peter K.

CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA

SOURCE: Helvetica Chimica Acta (2000), 83(8), 1825-1845

CODEN: HCACAV; ISSN: 0018-019X

PUBLISHER: Verlag Helvetica Chimica Acta

DOCUMENT TYPE: Journal

LANGUAGE: English

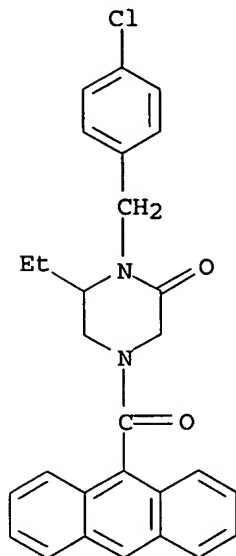
AB The development of a solution-phase approach to the rapid, parallel synthesis of highly functionalized piperazinones in only four steps starting from N-BOC-iminodiacetic acid is detailed. The efforts represent the extension of the solution-phase synthesis of combinatorial libraries from N-BOC-iminodiacetic acid to non-amide-based libraries where simple liquid-liquid extns. are employed to purify all reaction products. This methodol. was applied to the synthesis of a diverse 150-member library with substituents in three positions of the piperazinone core. Screening results from a luciferase reporter assay indicate that a number of library members are novel repressors of LEF-1/ $\beta$ -catenin-mediated transcription, and may be effective agents against colorectal tumors. Two secondary libraries (100 members each) designed from these lead structures were synthesized and screened, providing addnl. active agents and insight into key structure-activity relationships in the series. These compds. represent only the second class of small mols. which repress transcription of reporter genes containing LEF-1 responsive elements, and the first group not based on DNA minor-groove-binding agents.

IT 305327-53-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of non-amide-based combinatorial libraries derived from N-BOC-iminodiacetic acid and solution-phase synthesis of piperazinone libraries with activity against lymphoid-enhancer factor-1/ $\beta$ -

catenin-mediated transcription)  
 RN 305327-53-1 HCAPLUS  
 CN Piperazinone, 4-(9-anthracenylcarbonyl)-1-[(4-chlorophenyl)methyl]-6-ethyl-  
 (9CI) (CA INDEX NAME)



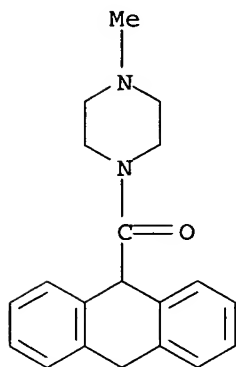
REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1969:501882 HCAPLUS  
 DOCUMENT NUMBER: 71:101882  
 TITLE: 9-(4-Methylpiperazino)methyl-9,10-dihydroanthracene  
 and similar compounds active on the central nervous  
 system  
 PATENT ASSIGNEE(S): Societe des usines chimiques de Rhone-Poulenc  
 SOURCE: Fr. M., 3 pp.  
 CODEN: FMXXAJ  
 DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 5432		19671113	FR	19660404

GI For diagram(s), see printed CA Issue.  
 AB I (R = 4-methyl-1-piperazinyl) is prepared by the reduction of  
 9-[(4-methyl-1-piperazinyl) carbonyl]-9,10-dihydroanthracene (II) with  
 LiAlH<sub>4</sub>. I (R = 4-methyl-1-piperazinyl) (m. 94-5°), I(R = NH<sub>2</sub>) (m.  
 92-3°, HCl salt m. 285-90°, allotropic form m. 76-7°  
 with HCl salt m. 280-5°), I(R = Me<sub>2</sub>N) (HCl salt m.  
 230-240°), and I(R = 4-benzyl-1-piperazinyl) (m. 116°) are  
 useful (adult dosage 5-200 mg./day) as tranquilizers, antidepressants,  
 anticonvulsants, anti-Parkinsonians, antihistamines, and antiserotonins.  
 Thus, a suspension of 0.8 g. LiAlH<sub>4</sub> in 60 ml. Et<sub>2</sub>O was treated slowly with  
 2.15 g. II, refluxed 2 hrs., cooled, and treated slowly with H<sub>2</sub>O 0.95, 5N  
 soda solution 0.7, and H<sub>2</sub>O 3.1 ml. to give 1.47 g. I (R =

4-methyl-1-piperazinyl).  
 IT 22063-98-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 22063-98-5 HCAPLUS  
 CN Piperazine, 1-(9,10-dihydro-9-anthroyl)-4-methyl- (8CI) (CA INDEX NAME)



L12 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1969:37552 HCAPLUS  
 DOCUMENT NUMBER: 70:37552  
 TITLE: Anthracene derivatives  
 INVENTOR(S): Fouche, Jean C. L.  
 PATENT ASSIGNEE(S): Societe des usines chimiques de Rhone-Poulenc  
 SOURCE: Fr., 5 pp.  
 CODEN: FRXXAK  
 DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1505351		19671215	FR	19660106

OTHER SOURCE(S): MARPAT 70:37552

GI For diagram(s), see printed CA Issue.

AB Novel derivs. (I) of 9,10-dihydroanthracene are prepared Thus, 68.5 g. LiAlH<sub>4</sub> in 1 l. anhydrous tetrahydrofuran was treated with 133.8 g. 10-hydroximinodibenzo[a,d]cycloheptadiene in 1.2 l. tetrahydrofuran in 25 min. with rise of temperature from 25 to 60° and the mixture refluxed 8 hrs., the cooled solution (ice bath) treated successively with 90.5 ml. H<sub>2</sub>O, 59 ml. 5N NaOH, and 264 ml. H<sub>2</sub>O; the residue on filtration washed with 2.5 l. tetrahydrofuran and 700 ml. CH<sub>2</sub>Cl<sub>2</sub>, the oily residue on evaporation taken up in 700 ml. Et<sub>2</sub>O; extracted with 650 ml. aqueous 2N MeSO<sub>3</sub>H, the acid solution washed with 400 ml. Et<sub>2</sub>O, made alkaline with 180 ml. 10N NaOH, the oily product extracted with 900 ml. Et<sub>2</sub>O, washed to neutrality with 1.6 l. H<sub>2</sub>O, the dried extract evaporated, the oily residue (68 g.) taken up in 200 ml. absolute alc., treated with 78 ml. dry HCl-absolute alc. (4.2 moles HCl/l. EtOH), and cooled 2 hrs. at 5° to give 57.3 g. I.HCl (Z = CH<sub>2</sub>NH<sub>2</sub>), m. 285-90°; free base (II) m. 92-3° or 76-8°. II was also prepared from I (Z = tosyloxymethyl) and NH<sub>3</sub>. Treatment of II with HCHO and HCO<sub>2</sub>H gave I.HCl (Z = Me<sub>2</sub>NCH<sub>2</sub>), m. 230-40°, also prepared by LiAlH<sub>4</sub> reduction of I (Z =



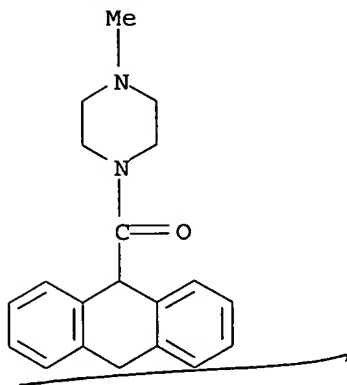
Me<sub>2</sub>NCO), m. 128-30°. LiAlH<sub>4</sub> reduction of I (Z = 4-methylpiperazinocarbonyl), m. 143-5°, gave I (Z = 4-methylpiperazinomethyl), m. 94-5°, also prepared from I. HCl (Z = CH<sub>2</sub>NH<sub>2</sub>) and (ClCH<sub>2</sub>CH<sub>2</sub>)<sub>2</sub>NMe·HCl. Similarly was prepared I (Z = 4-benzylpiperazinomethyl), m. 116°. I act as tranquilizers, antidepressants, anticonvulsants, antiparkinson agents, antihistaminic, and antiserotonin remedies. They are nontoxic as bases, salts, or quaternary ammonium compds. in the doses employed.

IT 22063-98-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 22063-98-5 HCAPLUS

CN Piperazine, 1-(9,10-dihydro-9-anthroyl)-4-methyl- (8CI) (CA INDEX NAME)



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FILE 'REGISTRY' ENTERED AT 16:56:25 ON 13 MAR 2006

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DICTIONARY FILE UPDATES: 12 MAR 2006 HIGHEST RN 876514-29-3

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* The CA roles and document type information have been removed from *
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* available and contains the CA role and document type information.  *
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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

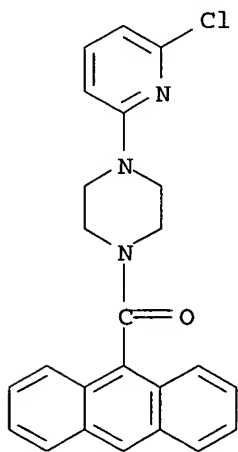
<http://www.cas.org/ONLINE/UG/regprops.html>

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L11 ANSWER 1 OF 18 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 848084-64-0 REGISTRY  
ED Entered STN: 07 Apr 2005  
CN Piperazine, 1-(9-anthracenylcarbonyl)-4-(6-chloro-2-pyridinyl)- (9CI) (CA INDEX NAME)  
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LC STN Files: CA, CAPLUS, TOXCENTER



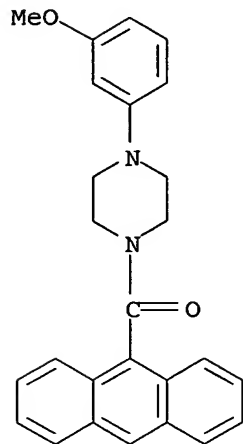
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1 REFERENCES IN FILE CA (1907 TO DATE)  
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REFERENCE 1: 142:309180

L11 ANSWER 2 OF 18 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 848084-63-9 REGISTRY  
ED Entered STN: 07 Apr 2005  
CN Piperazine, 1-(9-anthracenylcarbonyl)-4-(3-methoxyphenyl)- (9CI) (CA INDEX NAME)

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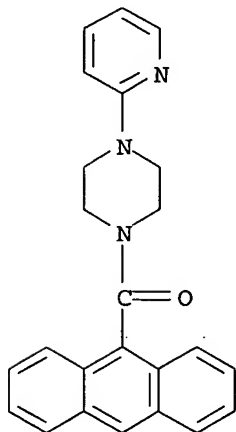


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1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 142:309180

L11 ANSWER 3 OF 18 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 647854-40-8 REGISTRY  
ED Entered STN: 09 Feb 2004  
CN Piperazine, 1-(9-anthracenylcarbonyl)-4-(2-pyridinyl)- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C24 H21 N3 O  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



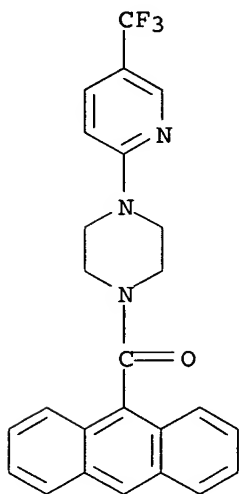
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2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:146164

REFERENCE 2: 140:111430

L11 ANSWER 4 OF 18 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 647854-39-5 REGISTRY  
ED Entered STN: 09 Feb 2004  
CN Piperazine, 1-(9-anthracenylcarbonyl)-4-[5-(trifluoromethyl)-2-pyridinyl]-  
(9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C25 H20 F3 N3 O  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



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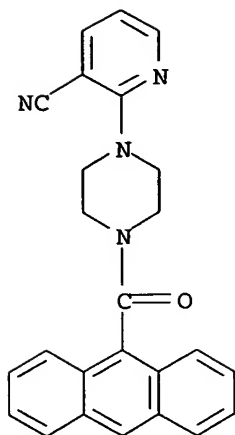
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REFERENCE 1: 140:146164

REFERENCE 2: 140:111430

L11 ANSWER 5 OF 18 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 647854-38-4 REGISTRY  
ED Entered STN: 09 Feb 2004  
CN Piperazine, 1-(9-anthracenylcarbonyl)-4-(3-cyano-2-pyridinyl)- (9CI) (CA  
INDEX NAME)  
FS 3D CONCORD  
MF C25 H20 N4 O  
SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:146164

REFERENCE 2: 140:111430

L11 ANSWER 6 OF 18 REGISTRY COPYRIGHT 2006 ACS on STN

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ED Entered STN: 09 Feb 2004

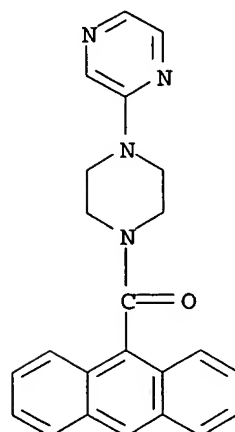
CN Piperazine, 1-(9-anthracenylcarbonyl)-4-pyrazinyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C23 H20 N4 O

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LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



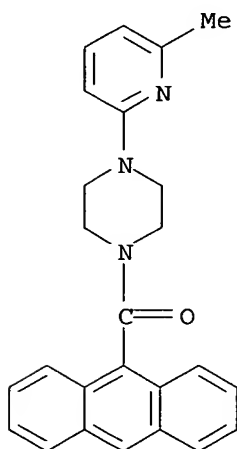
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REFERENCE 2: 140:111430

L11 ANSWER 7 OF 18 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 647854-36-2 REGISTRY  
ED Entered STN: 09 Feb 2004  
CN Piperazine, 1-(9-anthracenylcarbonyl)-4-(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C25 H23 N3 O  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



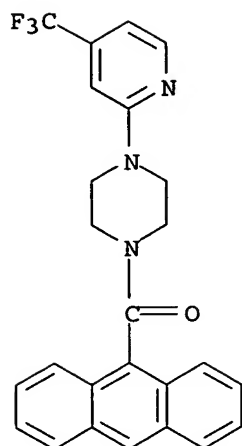
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:146164

REFERENCE 2: 140:111430

L11 ANSWER 8 OF 18 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 647854-35-1 REGISTRY  
ED Entered STN: 09 Feb 2004  
CN Piperazine, 1-(9-anthracenylcarbonyl)-4-[4-(trifluoromethyl)-2-pyridinyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C25 H20 F3 N3 O  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:146164

REFERENCE 2: 140:111430

L11 ANSWER 9 OF 18 REGISTRY COPYRIGHT 2006 ACS on STN

RN 647854-34-0 REGISTRY

ED Entered STN: 09 Feb 2004

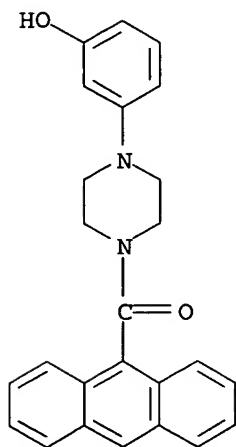
CN Piperazine, 1-(9-anthracenylcarbonyl)-4-(3-hydroxyphenyl)- (9CI) (CA  
INDEX NAME)

FS 3D CONCORD

MF C25 H22 N2 O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



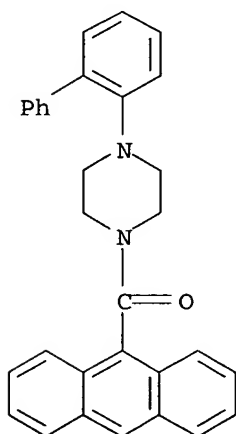
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:146164

REFERENCE 2: 140:111430

L11 ANSWER 10 OF 18 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 647854-33-9 REGISTRY  
ED Entered STN: 09 Feb 2004  
CN Piperazine, 1-(9-anthracenylcarbonyl)-4-[1,1'-biphenyl]-2-yl- (9CI) (CA  
INDEX NAME)  
FS 3D CONCORD  
MF C31 H26 N2 O  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

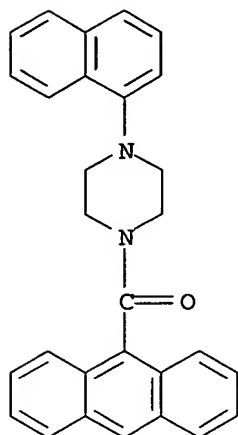
2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:146164

REFERENCE 2: 140:111430

L11 ANSWER 11 OF 18 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 647854-32-8 REGISTRY  
ED Entered STN: 09 Feb 2004  
CN Piperazine, 1-(9-anthracenylcarbonyl)-4-(1-naphthalenyl)- (9CI) (CA INDEX  
NAME)  
FS 3D CONCORD  
MF C29 H24 N2 O  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL





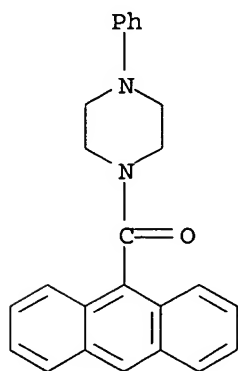
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:146164

REFERENCE 2: 140:111430

L11 ANSWER 12 OF 18 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 647854-31-7 REGISTRY  
ED Entered STN: 09 Feb 2004  
CN Piperazine, 1-(9-anthracenylcarbonyl)-4-phenyl- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C25 H22 N2 O  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



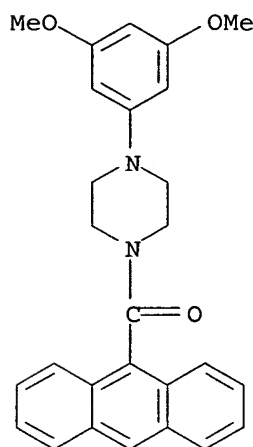
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:146164

REFERENCE 2: 140:111430

L11 ANSWER 13 OF 18 REGISTRY COPYRIGHT 2006 ACS on STN  
 RN 647854-30-6 REGISTRY  
 ED Entered STN: 09 Feb 2004  
 CN Piperazine, 1-(9-anthracenylcarbonyl)-4-(3,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C27 H26 N2 O3  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



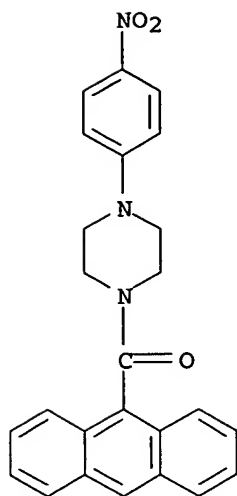
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:146164

REFERENCE 2: 140:111430

L11 ANSWER 14 OF 18 REGISTRY COPYRIGHT 2006 ACS on STN  
 RN 647854-29-3 REGISTRY  
 ED Entered STN: 09 Feb 2004  
 CN Piperazine, 1-(9-anthracenylcarbonyl)-4-(4-nitrophenyl)- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C25 H21 N3 O3  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:146164

REFERENCE 2: 140:111430

L11 ANSWER 15 OF 18 REGISTRY COPYRIGHT 2006 ACS on STN

RN 591781-16-7 REGISTRY

ED Entered STN: 24 Sep 2003

CN Morpholine, 4-[[[(1R,3S)-3-[4-(9-anthracenylcarbonyl)-1-piperazinyl]cyclohexyl]carbonyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN (Anthracen-9-yl) [4-[(1S,3R)-3-[(morpholin-4-yl)carbonyl]cyclohexyl]piperazin-1-yl]methanone

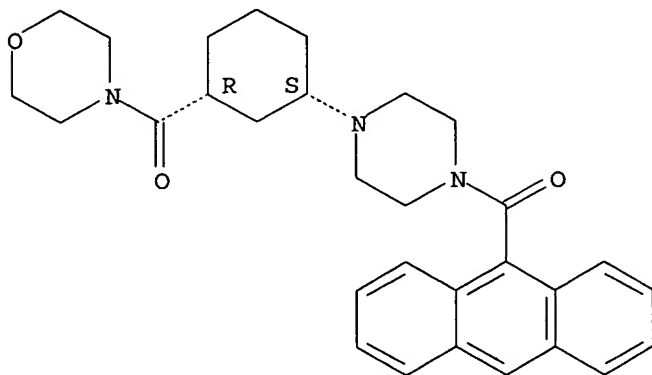
FS STEREOSEARCH

MF C30 H35 N3 O3

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

Absolute stereochemistry.



## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:230625

L11 ANSWER 16 OF 18 REGISTRY COPYRIGHT 2006 ACS on STN

RN 591781-15-6 REGISTRY

ED Entered STN: 24 Sep 2003

CN Morpholine, 4-[[[(1R,3R)-3-[4-(9-anthracenylcarbonyl)-1-piperazinyl]cyclohexyl]carbonyl]- (9CI) (CA INDEX NAME)

## OTHER NAMES:

CN (Anthracen-9-yl) [4-[(1R,3R)-3-[(morpholin-4-yl)carbonyl]cyclohexyl]piperazin-1-yl]methanone

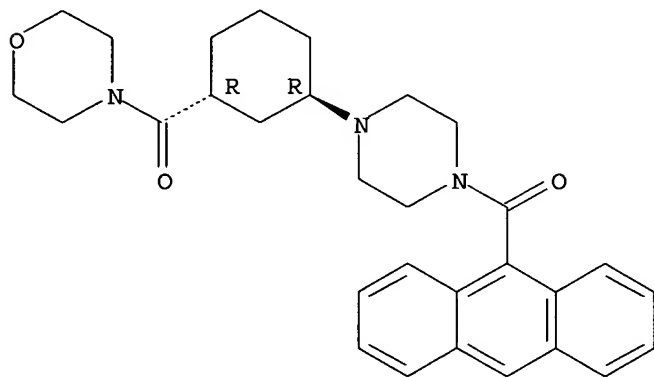
FS STEREOSEARCH

MF C30 H35 N3 O3

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

Absolute stereochemistry.



## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:230625

L11 ANSWER 17 OF 18 REGISTRY COPYRIGHT 2006 ACS on STN

RN 305327-53-1 REGISTRY

ED Entered STN: 30 Nov 2000

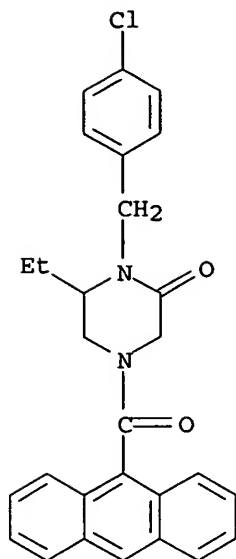
CN Piperazinone, 4-(9-anthracenylcarbonyl)-1-[(4-chlorophenyl)methyl]-6-ethyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C28 H25 Cl N2 O2

SR CA

LC STN Files: CA, CAPLUS

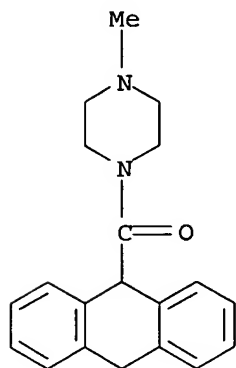


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 133:350193

L11 ANSWER 18 OF 18 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 22063-98-5 REGISTRY  
ED Entered STN: 16 Nov 1984  
CN Piperazine, 1-(9,10-dihydro-9-anthroyl)-4-methyl- (8CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C20 H22 N2 O  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, TOXCENTER  
(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 71:101882

REFERENCE 2: 70:37552

=> => fil beil

FILE 'BEILSTEIN' ENTERED AT 17:02:58 ON 13 MAR 2006

COPYRIGHT (c) 2006 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften  
licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE LAST UPDATED ON JANUARY 17, 2006

FILE COVERS 1771 TO 2005.

\*\*\* FILE CONTAINS 9,428,406 SUBSTANCES \*\*\*

>>>PLEASE NOTE: Reaction Data and substance data are stored in  
separate documents and can not be searched together in one query.  
Reaction data for BEILSTEIN compounds may be displayed  
immediately with the display codes PRE (preparations) and REA  
(reactions). A substance answer set retrieved after the search  
for a chemical name, a compounds with available reaction  
information by combining with PRE/FA, REA/FA or more generally  
with RX/FA. The BEILSTEIN Registry Number (BRN) is the link  
between a BEILSTEIN compound and belonging reactions. For mo  
detailed reaction searches BRNs can be searched as reaction  
partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

\*\*\*\*\*  
\* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. \*  
\* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE \*  
\* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE \*  
\* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. \*  
\* FOR PRICE INFORMATION SEE HELP COST \*  
\*\*\*\*\*

#### NEW

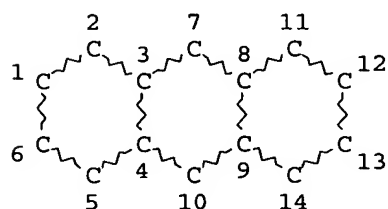
\* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE  
SEARCHED, SELECTED AND TRANSFERRED.  
\* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES,  
ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A  
COMPOUND AT A GLANCE.

=>

=>

=> d stat que 114

L5 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

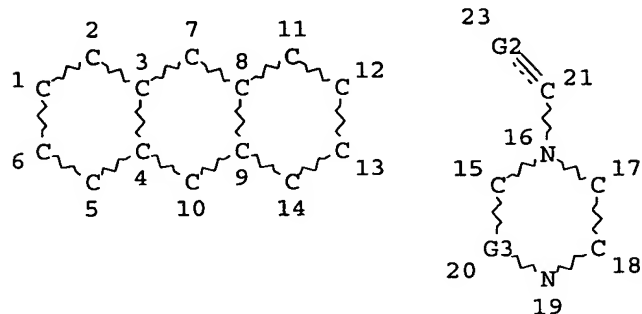
RSPEC I

NUMBER OF NODES IS 14

## STEREO ATTRIBUTES: NONE

L7 118852 SEA FILE=REGISTRY SSS FUL L5

L8 STR



VAR G2=O/S

REP G3=(1-4) C

## NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

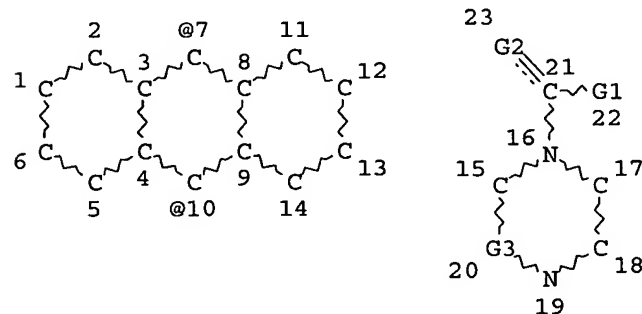
RSPEC 16

NUMBER OF NODES IS 22

## STEREO ATTRIBUTES: NONE

L9 157 SEA FILE=REGISTRY SUB=L7 SSS FUL L8

L10 STR



VAR G1=7/10

VAR G2=O/S

REP G3=(1-4) C

## NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RSPEC 15

NUMBER OF NODES IS 23

## STEREO ATTRIBUTES: NONE

L11 18 SEA FILE=REGISTRY SUB=L9 SSS FUL L10

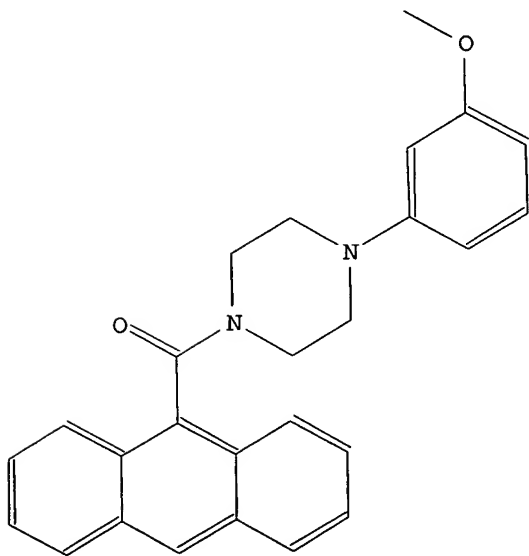
L13 4 SEA FILE=BEILSTEIN SSS FUL L10  
 L14 3 SEA FILE=BEILSTEIN ABB=ON PLU=ON L13 NOT L11

=>

=> d brn cn mf fw str pharm rx l14 1-3

L14 ANSWER 1 OF 3 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Beilstein Records (BRN):	10031190
Chemical Name (CN):	anthracen-9-yl-<4-(3-methoxy-phenyl)-piperazin-1-yl>-methanone
Autonom Name (AUN):	anthracen-9-yl-<4-(3-methoxy-phenyl)-piperazin-1-yl>-methanone
Molecular Formula (MF):	C26 H24 N2 O2
Molecular Weight (MW):	396.49



#### Pharmacological Data:

##### PHARM

Effect (.E):	cytotoxicity
Species or Test-System (.SP):	murine leukemia L1210 cells
Kind of Dosing (.KD):	title comp. dissolved in DMSO added
Method, Remarks (.MR):	cells and title comp. incubated for 48 h; XTT assay used to determine proliferation; IC50-values obtained by nonlinear regression
Further Details (.FD):	XTT: sodium 3'-<1-(phenyl-amino-carbonyl)-3,4-tetrazolium>-bis(4-methoxy-6-nitro)benzene sulfonic acid hydrate; reference comp. paclitaxel, vincristine: IC50 = 0.06, 0.02 .my.mol/l, respectively IC50 0.48 .my.mol/l
Type (.TYP):	
Value of Type (.V):	



## Reference(s):

1. Gerlach, Matthias; Claus, Eckhard; Baasner, Silke; Mueller, Gilbert; Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel, Juergen, Arch. Pharm. (Weinheim Ger.), CODEN: ARPMAS, 337(12), <2004>, 695 - 703; BABS-6492751

## PHARM

Effect (.E): cytotoxicity  
 Species or Test-System (.SP): murine leukemia P388 cells  
 Kind of Dosing (.KD): title comp. dissolved in DMSO added  
 Method, Remarks (.MR): cells and title comp. incubated for 48 h;  
 XTT assay used to determine proliferation;  
 IC50-values obtained by nonlinear regression  
 Further Details (.FD): XTT: sodium 3'-(1-(phenyl-amino-carbonyl)-3,4-tetrazolium>-bis(4-methoxy-6-nitro)benzene sulfonic acid hydrate;  
 reference comp. paclitaxel, vincristine:  
 IC50 = 0.04, 0.004 .my.mol/l, respectively  
 Type (.TYP): IC50  
 Value of Type (.V): 0.28 .my.mol/l  
 Reference(s):  
 1. Gerlach, Matthias; Claus, Eckhard; Baasner, Silke; Mueller, Gilbert; Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel, Juergen, Arch. Pharm. (Weinheim Ger.), CODEN: ARPMAS, 337(12), <2004>, 695 - 703; BABS-6492751

## PHARM

Effect (.E): cytotoxicity  
 Species or Test-System (.SP): murine leukemia P388ADR cells  
 Kind of Dosing (.KD): title comp. dissolved in DMSO added  
 Method, Remarks (.MR): cells and title comp. incubated for 48 h;  
 XTT assay used to determine proliferation;  
 IC50-values obtained by nonlinear regression  
 Further Details (.FD): ADR resistant cells used; XTT: sodium 3'-(1-(phenyl-amino-carbonyl)-3,4-tetrazolium>-bis(4-methoxy-6-nitro)benzene sulfonic acid hydrate; reference comp. paclitaxel, vincristine: IC50 = >5, 0.93 .my.mol/l, respectively  
 Type (.TYP): IC50  
 Value of Type (.V): 0.25 .my.mol/l  
 Reference(s):  
 1. Gerlach, Matthias; Claus, Eckhard; Baasner, Silke; Mueller, Gilbert; Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel, Juergen, Arch. Pharm. (Weinheim Ger.), CODEN: ARPMAS, 337(12), <2004>, 695 - 703; BABS-6492751

## PHARM

Effect (.E): cytotoxicity  
 Species or Test-System (.SP): murine leukemia L1210VCR cells  
 Kind of Dosing (.KD): title comp. dissolved in DMSO added  
 Method, Remarks (.MR): cells and title comp. incubated for 48 h;  
 XTT assay used to determine proliferation;  
 IC50-values obtained by nonlinear regression  
 Further Details (.FD): VCR resistant cells used; XTT: sodium 3'-(1-(phenyl-amino-carbonyl)-3,4-tetrazolium>-bis(4-methoxy-6-nitro)benzene sulfonic acid hydrate; reference comp. paclitaxel and vincristine: IC50 > 5 .my.mol/l, respectively

Type (.TYP): IC50  
 Value of Type (.V): 0.37 .my.mol/l  
 Reference(s):  
 1. Gerlach, Matthias; Claus, Eckhard; Baasner, Silke; Mueller, Gilbert; Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel, Juergen, Arch. Pharm. (Weinheim Ger.), CODEN: ARPMAS, 337(12), <2004>, 695 - 703; BABS-6492751

## PHARM

Effect (.E): cytotoxicity  
 Species or Test-System (.SP): rat leukemia LT12MDR subline cells  
 Kind of Dosing (.KD): title comp. dissolved in DMSO added  
 Method, Remarks (.MR): cells and title comp. incubated for 48 h; XTT assay used to determine proliferation; IC50-values obtained by nonlinear regression  
 Further Details (.FD): multi drug resistant cells used; XTT: sodium 3'-<1-(phenyl-amino-carbonyl)-3,4-tetrazolium>-bis(4-methoxy-6-nitro)benzene sulfonic acid hydrate; reference comp. paclitaxel, vincristine: IC50 = 0.4, 0.134 .my.mol/l, respectively  
 Type (.TYP): IC50  
 Value of Type (.V): 0.26 .my.mol/l  
 Reference(s):  
 1. Gerlach, Matthias; Claus, Eckhard; Baasner, Silke; Mueller, Gilbert; Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel, Juergen, Arch. Pharm. (Weinheim Ger.), CODEN: ARPMAS, 337(12), <2004>, 695 - 703; BABS-6492751

## PHARM

Effect (.E): cytotoxicity  
 Species or Test-System (.SP): rat leukemia LT12 cells  
 Kind of Dosing (.KD): title comp. dissolved in DMSO added  
 Method, Remarks (.MR): cells and title comp. incubated for 48 h; XTT assay used to determine proliferation; IC50-values obtained by nonlinear regression  
 Further Details (.FD): XTT: sodium 3'-<1-(phenyl-amino-carbonyl)-3,4-tetrazolium>-bis(4-methoxy-6-nitro)benzene sulfonic acid hydrate; reference comp. paclitaxel, vincristine: IC50 = 0.01, 0.002 .my.mol/l, respectively  
 Type (.TYP): IC50  
 Value of Type (.V): 0.32 .my.mol/l  
 Reference(s):  
 1. Gerlach, Matthias; Claus, Eckhard; Baasner, Silke; Mueller, Gilbert; Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel, Juergen, Arch. Pharm. (Weinheim Ger.), CODEN: ARPMAS, 337(12), <2004>, 695 - 703; BABS-6492751

## PHARM

Effect (.E): protein binding  
 Species or Test-System (.SP): biotin-labeled tubulin  
 Kind of Dosing (.KD): title comp. dissolved in DMSO added  
 Method, Remarks (.MR): diluted title comp. and <3H>colchicine transferred to a 96-well isoplate, incubated with buffer and tubulin; streptavidin-coated yttrium SPA beads added; bound radioactivity determined using scintillation counter; IC50 obtained by nonlinear regression  
 Further Details (.FD): reconstituted biotin-labeled tubulin

(T333, Cytoskeleton) used for  
<3H>colchicine competition assay;  
reference comp. colchicine: IC50 = 1.26  
.my.mol/ml

Type (.TYP): IC50  
Value of Type (.V): 4.51 .my.mol/l  
Reference(s):

1. Gerlach, Matthias; Claus, Eckhard; Baasner, Silke; Mueller, Gilbert; Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel, Juergen, Arch. Pharm. (Weinheim Ger.), CODEN: ARPMAS, 337(12), <2004>, 695 - 703; BABS-6492751

## PHARM

Effect (.E): protein polymerisation; inhibition of  
Species or Test-System (.SP): bovine brain tubulin  
Kind of Dosing (.KD): title comp. dissolved in DMSO  
Method, Remarks (.MR): tubulin heterodimers incubated with title  
comp. in 96-well half area plates; tubulin  
polymerization determined at 340 nm;  
inhib. calculated from areas under the  
curves

Further Details (.FD): lyophilized bovine brain tubulin (2 mg/ml  
ML113-MAP rich or 5 mg/ml TL238-MAP free)  
used; MAP: microtubule associated  
proteine; reference comp. paclitaxel,  
colchicine: IC50 = >10, 2.6 .my.mol/l,  
respectively

Type (.TYP): IC50  
Value of Type (.V): 5.59 .my.mol/l  
Reference(s):

1. Gerlach, Matthias; Claus, Eckhard; Baasner, Silke; Mueller, Gilbert; Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel, Juergen, Arch. Pharm. (Weinheim Ger.), CODEN: ARPMAS, 337(12), <2004>, 695 - 703; BABS-6492751

## PHARM

Effect (.E): cytotoxicity  
Species or Test-System (.SP): non-small cell lung cancer NCI-H460 cells  
Kind of Dosing (.KD): title comp. dissolved in DMSO added  
Method, Remarks (.MR): cells and title comp. incubated for 48 h;  
XTT assay used to determine proliferation;  
IC50-values obtained by nonlinear  
regression

Further Details (.FD): XTT: sodium 3'-<1-(phenyl-amino-carbonyl)-  
3,4-tetrazolium>-bis(4-methoxy-6-  
nitro)benzene sulfonic acid hydrate;  
reference comp. paclitaxel, colchicine:  
IC50 = 0.01, 0.07 .my.mol/l, respectively

Type (.TYP): IC50  
Value of Type (.V): 0.26 .my.mol/l  
Reference(s):

1. Gerlach, Matthias; Claus, Eckhard; Baasner, Silke; Mueller, Gilbert; Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel, Juergen, Arch. Pharm. (Weinheim Ger.), CODEN: ARPMAS, 337(12), <2004>, 695 - 703; BABS-6492751

## PHARM

Effect (.E): cytotoxicity  
Species or Test-System (.SP): CNS cancer (glioma) SF268 cells  
Kind of Dosing (.KD): title comp. dissolved in DMSO added  
Method, Remarks (.MR): cells and title comp. incubated for 48 h;  
XTT assay used to determine proliferation;  
IC50-values obtained by nonlinear

Further Details (.FD): regression  
 XTT: sodium 3'-<1-(phenyl-amino-carbonyl)-  
 3,4-tetrazolium>-bis(4-methoxy-6-  
 nitro)benzene sulfonic acid hydrate;  
 reference comp. paclitaxel, colchicine:  
 IC50 = 0.01, 0.05 .my.mol/l, respectively  
 Type (.TYP): IC50  
 Value of Type (.V): 0.15 .my.mol/l  
 Reference(s):  
 1. Gerlach, Matthias; Claus, Eckhard; Baasner, Silke; Mueller, Gilbert;  
 Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel,  
 Juergen, Arch. Pharm. (Weinheim Ger.), CODEN: ARPMAS, 337(12), <2004>,  
 695 - 703; BABS-6492751

## PHARM

Effect (.E): cytotoxicity  
 Species or Test-System (.SP): human ovarian carcinoma SKOV3 cells  
 Kind of Dosing (.KD): title comp. dissolved in DMSO added  
 Method, Remarks (.MR): cells and title comp. incubated for 48 h;  
 XTT assay used to determine proliferation;  
 IC50-values obtained by nonlinear  
 regression  
 Further Details (.FD): XTT: sodium 3'-<1-(phenyl-amino-carbonyl)-  
 3,4-tetrazolium>-bis(4-methoxy-6-  
 nitro)benzene sulfonic acid hydrate;  
 reference comp. paclitaxel, colchicine:  
 IC50 = 0.01, 0.05 .my.mol/l, respectively  
 Type (.TYP): IC50  
 Value of Type (.V): 0.13 .my.mol/l  
 Reference(s):  
 1. Gerlach, Matthias; Claus, Eckhard; Baasner, Silke; Mueller, Gilbert;  
 Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel,  
 Juergen, Arch. Pharm. (Weinheim Ger.), CODEN: ARPMAS, 337(12), <2004>,  
 695 - 703; BABS-6492751

## PHARM

Effect (.E): cytotoxicity  
 Species or Test-System (.SP): human cervix carcinoma KB/HeLa cells  
 Kind of Dosing (.KD): title comp. dissolved in DMSO added  
 Method, Remarks (.MR): cells and title comp. incubated for 48 h;  
 XTT assay used to determine proliferation;  
 IC50-values obtained by nonlinear  
 regression  
 Further Details (.FD): XTT: sodium 3'-<1-(phenyl-amino-carbonyl)-  
 3,4-tetrazolium>-bis(4-methoxy-6-  
 nitro)benzene sulfonic acid hydrate;  
 reference comp. paclitaxel, colchicine:  
 IC50 = 0.01, 0.03 .my.mol/l, respectively  
 Type (.TYP): IC50  
 Value of Type (.V): 0.14 .my.mol/l  
 Reference(s):  
 1. Gerlach, Matthias; Claus, Eckhard; Baasner, Silke; Mueller, Gilbert;  
 Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel,  
 Juergen, Arch. Pharm. (Weinheim Ger.), CODEN: ARPMAS, 337(12), <2004>,  
 695 - 703; BABS-6492751

## Reaction:

## RX

Reaction ID (.ID): 9894343  
 Reactant BRN (.RBRN): 1875336, 611157  
 Reactant (.RCT): anthracene-9-carboxylic acid,  
 1-(3-methoxy-phenyl)-piperazine

Product BRN (.PBRN): 10031190  
Product (.PRO): anthracen-9-yl-<4-(3-methoxy-phenyl)-piperazin-1-yl>-methanone  
No. of React. Details (.NVAR): 1

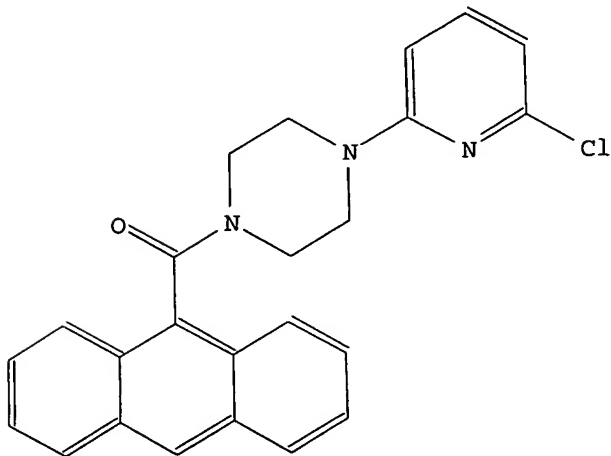
## Reaction Details:

RX

Reaction RID (.RID): 9894343.1  
Reaction Classification (.CL): Multistage  
Yield (.YDT): 9 percent (BRN=10031190)  
Nr. of Stages (.SNR): 2  
Stage 1  
Reagent (.RGT): N-cyclohexylcarbodiimide bound to N'-methyl polystyrene HL  
Solvent (.SOL): CH<sub>2</sub>Cl<sub>2</sub>  
Time (.TIM): 30 min  
Temperature (.T): 20 Cel  
Stage 2  
Stage reactant (.SRCT): 1-(3-methoxy-phenyl)-piperazine  
Stage Reactant BRN (.SRBRN): 611157  
Solvent (.SOL): CH<sub>2</sub>Cl<sub>2</sub>  
Time (.TIM): 16 hour(s)  
Temperature (.T): 20 Cel  
Reference(s):  
1. Gerlach, Matthias; Claus, Eckhard; Baasner, Silke; Mueller, Gilbert; Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel, Juergen, Arch. Pharm. (Weinheim Ger.), CODEN: ARPMAS, 337(12), <2004>, 695 - 703; BABS-6492751

L14 ANSWER 2 OF 3 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Beilstein Records (BRN): 10030053  
Chemical Name (CN): anthracen-9-yl-<4-(6-chloro-pyridin-2-yl)-piperazin-1-yl>-methanone  
Autonom Name (AUN): anthracen-9-yl-<4-(6-chloro-pyridin-2-yl)-piperazin-1-yl>-methanone  
Molecular Formula (MF): C<sub>24</sub> H<sub>20</sub> Cl N<sub>3</sub> O  
Molecular Weight (MW): 401.89



## Pharmacological Data:

## PHARM

Effect (.E): protein polymerisation; inhibition of  
 Species or Test-System (.SP): bovine brain tubulin  
 Kind of Dosing (.KD): title comp. dissolved in DMSO added  
 Method, Remarks (.MR): tubulin heterodimers incubated with title  
 comp. in 96-well half area plates; tubulin  
 polymerization determined at 340 nm;  
 inhib. calculated from areas under the  
 curves  
 Further Details (.FD): lyophilized bovine brain tubulin (2 mg/ml  
 ML113-MAP rich or 5 mg/ml TL238-MAP free)  
 used; MAP: microtubule associated  
 proteine; reference comp. paclitaxel,  
 colchicine: IC50 = >10, 2.6 .my.mol/l,  
 respectively  
 Type (.TYP): IC50  
 Value of Type (.V): 6.65 .my.mol/l  
 Reference(s):  
 1. Gerlach, Matthias; Claus, Eckhard; Baasner, Silke; Mueller, Gilbert;  
 Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel,  
 Juergen, Arch. Pharm. (Weinheim Ger.), CODEN: ARPMAS, 337(12), <2004>,  
 695 - 703; BABS-6492751

## PHARM

Effect (.E): cytotoxicity  
 Species or Test-System (.SP): non-small cell lung cancer NCI-H460 cells  
 Kind of Dosing (.KD): title comp. dissolved in DMSO added  
 Method, Remarks (.MR): cells and title comp. incubated for 48 h;  
 XTT assay used to determine proliferation;  
 IC50-values obtained by nonlinear  
 regression  
 Further Details (.FD): XTT: sodium 3'-(1-(phenyl-amino-carbonyl)-  
 3,4-tetrazolium)-bis(4-methoxy-6-  
 nitro)benzene sulfonic acid hydrate;  
 reference comp. paclitaxel, colchicine:  
 IC50 = 0.01, 0.07 .my.mol/l, respectively  
 Type (.TYP): IC50  
 Value of Type (.V): 0.7 .my.mol/l  
 Reference(s):  
 1. Gerlach, Matthias; Claus, Eckhard; Baasner, Silke; Mueller, Gilbert;  
 Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel,  
 Juergen, Arch. Pharm. (Weinheim Ger.), CODEN: ARPMAS, 337(12), <2004>,  
 695 - 703; BABS-6492751

## PHARM

Effect (.E): cytotoxicity  
 Species or Test-System (.SP): CNS cancer (glioma) SF268 cells  
 Kind of Dosing (.KD): title comp. dissolved in DMSO added  
 Method, Remarks (.MR): cells and title comp. incubated for 48 h;  
 XTT assay used to determine proliferation;  
 IC50-values obtained by nonlinear  
 regression  
 Further Details (.FD): XTT: sodium 3'-(1-(phenyl-amino-carbonyl)-  
 3,4-tetrazolium)-bis(4-methoxy-6-  
 nitro)benzene sulfonic acid hydrate;  
 reference comp. paclitaxel, colchicine:  
 IC50 = 0.01, 0.05 .my.mol/l, respectively  
 Type (.TYP): IC50  
 Value of Type (.V): 0.74 .my.mol/l

## Reference(s):

1. Gerlach, Matthias; Claus, Eckhard; Baasner, Silke; Mueller, Gilbert; Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel, Juergen, Arch. Pharm. (Weinheim Ger.), CODEN: ARPMAS, 337(12), <2004>, 695 - 703; BABS-6492751

## PHARM

Effect (.E): cytotoxicity  
 Species or Test-System (.SP): human ovarian carcinoma SKOV3 cells  
 Kind of Dosing (.KD): title comp. dissolved in DMSO added  
 Method, Remarks (.MR): cells and title comp. incubated for 48 h;  
 XTT assay used to determine proliferation;  
 IC50-values obtained by nonlinear regression  
 Further Details (.FD): XTT: sodium 3'-<1-(phenyl-amino-carbonyl)-3,4-tetrazolium>-bis(4-methoxy-6-nitro)benzene sulfonic acid hydrate;  
 reference comp. paclitaxel, colchicine:  
 IC50 = 0.01, 0.05 .my.mol/l, respectively  
 Type (.TYP): IC50  
 Value of Type (.V): 0.66 .my.mol/l  
 Reference(s):  
 1. Gerlach, Matthias; Claus, Eckhard; Baasner, Silke; Mueller, Gilbert; Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel, Juergen, Arch. Pharm. (Weinheim Ger.), CODEN: ARPMAS, 337(12), <2004>, 695 - 703; BABS-6492751

## PHARM

Effect (.E): cytotoxicity  
 Species or Test-System (.SP): human cervix carcinoma KB/HeLa cells  
 Kind of Dosing (.KD): title comp. dissolved in DMSO added  
 Method, Remarks (.MR): cells and title comp. incubated for 48 h;  
 XTT assay used to determine proliferation;  
 IC50-values obtained by nonlinear regression  
 Further Details (.FD): XTT: sodium 3'-<1-(phenyl-amino-carbonyl)-3,4-tetrazolium>-bis(4-methoxy-6-nitro)benzene sulfonic acid hydrate;  
 reference comp. paclitaxel, colchicine:  
 IC50 = 0.01, 0.03 .my.mol/l, respectively  
 Type (.TYP): IC50  
 Value of Type (.V): 1.14 .my.mol/l  
 Reference(s):  
 1. Gerlach, Matthias; Claus, Eckhard; Baasner, Silke; Mueller, Gilbert; Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel, Juergen, Arch. Pharm. (Weinheim Ger.), CODEN: ARPMAS, 337(12), <2004>, 695 - 703; BABS-6492751

## Reaction:

## RX

Reaction ID (.ID): 9898858  
 Reactant BRN (.RBRN): 1875336, 783165  
 Reactant (.RCT): anthracene-9-carboxylic acid,  
 1-(6-chloro-pyridin-2-yl)-piperazine  
 Product BRN (.PBRN): 10030053  
 Product (.PRO): anthracen-9-yl-<4-(6-chloro-pyridin-2-yl)-piperazin-1-yl>-methanone  
 No. of React. Details (.NVAR): 1

## Reaction Details:

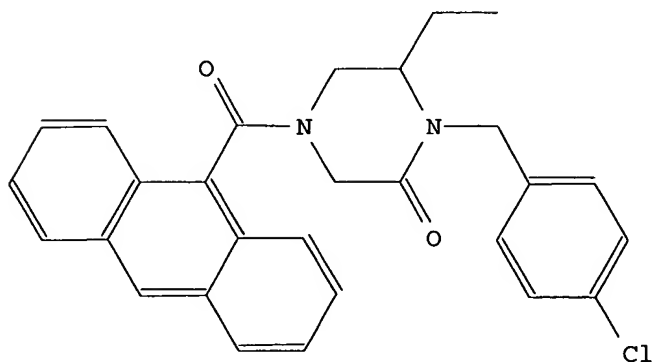
## RX

Reaction RID (.RID): 9898858.1

Reaction Classification (.CL): Multistage  
 Yield (.YDT): 11 percent (BRN=10030053)  
 Nr. of Stages (.SNR): 2  
 Stage 1  
 Reagent (.RGT): N-cyclohexylcarbodiimide bound to  
 N'-methyl polystyrene HL  
 Solvent (.SOL): CH<sub>2</sub>Cl<sub>2</sub>  
 Time (.TIM): 30 min  
 Temperature (.T): 20 Cel  
 Stage 2  
 Stage reactant (.SRCT): 1-(6-chloro-pyridin-2-yl)-piperazine  
 Stage Reactant BRN (.SRBRN): 783165  
 Solvent (.SOL): CH<sub>2</sub>Cl<sub>2</sub>  
 Time (.TIM): 16 hour(s)  
 Temperature (.T): 20 Cel  
 Reference(s):  
 1. Gerlach, Matthias; Claus, Eckhard; Baasner, Silke; Mueller, Gilbert;  
 Polymeropoulos, Emmanuel; Schmidt, Peter; Guenther, Eckhard; Engel,  
 Juergen, Arch. Pharm. (Weinheim Ger.), CODEN: ARPMAS, 337(12), <2004>,  
 695 - 703; BABS-6492751

## L14 ANSWER 3 OF 3 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Beilstein Records (BRN): 8730424  
 Chemical Name (CN): 4-(anthracene-9-carbonyl)-1-(4-chloro-  
 benzyl)-6-ethyl-piperazin-2-one  
 Autonom Name (AUN): 4-(anthracene-9-carbonyl)-1-(4-chloro-  
 benzyl)-6-ethyl-piperazin-2-one  
 Molecular Formula (MF): C<sub>28</sub> H<sub>25</sub> Cl N<sub>2</sub> O<sub>2</sub>  
 Molecular Weight (MW): 456.97



## Pharmacological Data:

## PHARM

Effect (.E): inhibition of gene transcription  
 Species or Test-System (.SP): colon-cancer cell line (SW480)  
 Concentration (.C): 10 .my.mol/l  
 Method, Remarks (.MR): cells transfected with DNA (TOPFLASH 6  
 .my.g); after 24 h treated with title  
 comp.; after 48 h determined repression of  
 LEF-1/ $\beta$ -catenin-mediated  
 transcription in luciferase promoter  
 region (TOPFLASH) by measuring luciferase



activity (luminescence)  
 Further Details (.FD): TOPFLASH contains four copies of the LEF-1 (lymphoid-enhancer binding factor) binding site (CCTTTGATC) upstream from the promoter that augment transcription  
 Results (.RE): < 1.2-fold repression of transcription  
 Reference(s):  
 1. Boger, Dale L.; Goldberg, Joel; Satoh, Shigeki; Ambroise, Yves; Cohen, Steven B.; Vogt, Peter K., Helv.Chim.Acta, CODEN: HCACAV, 83(8), <2000>, 1825 - 1845; BABS-6258794

## Reaction:

RX

Reaction ID (.ID): 8678222  
 Reactant BRN (.RBRN): 8692887, 1875336  
 Reactant (.RCT): 1-(4-chloro-benzyl)-6-ethyl-piperazin-2-one, anthracene-9-carboxylic acid  
 Product BRN (.PBRN): 8730424  
 Product (.PRO): 4-(anthracene-9-carbonyl)-1-(4-chloro-benzyl)-6-ethyl-piperazin-2-one  
 No. of React. Details (.NVAR): 1

## Reaction Details:

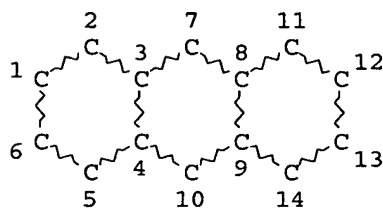
RX

Reaction RID (.RID): 8678222.1  
 Reaction Classification (.CL): Preparation  
 Reagent (.RGT): EtN(i-Pr)<sub>2</sub>, EDCI  
 Reaction Type (.TYP): Acylation  
 Reference(s):  
 1. Boger, Dale L.; Goldberg, Joel; Satoh, Shigeki; Ambroise, Yves; Cohen, Steven B.; Vogt, Peter K., Helv.Chim.Acta, CODEN: HCACAV, 83(8), <2000>, 1825 - 1845; BABS-6258794

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L5

STR



## NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

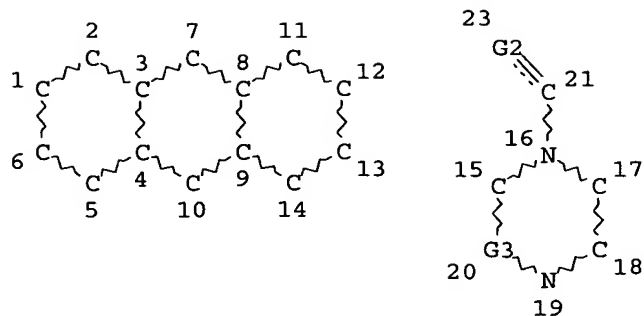
RSPEC I

NUMBER OF NODES IS 14

## STEREO ATTRIBUTES: NONE

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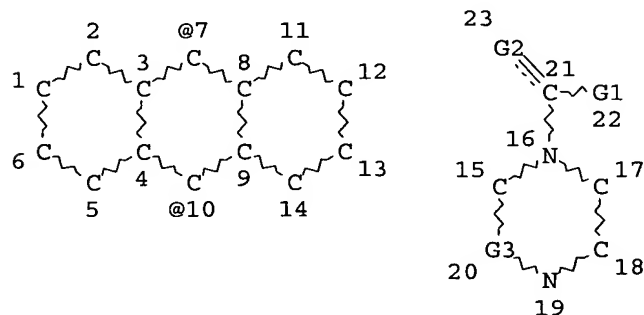
L8 STR



VAR G2=O/S  
 REP G3=(1-4) C  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RSPEC 16  
 NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE  
 L9 157 SEA FILE=REGISTRY SUB=L7 SSS FUL L8  
 L10 STR



VAR G1=7/10  
 VAR G2=O/S  
 REP G3=(1-4) C  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RSPEC 15  
 NUMBER OF NODES IS 23

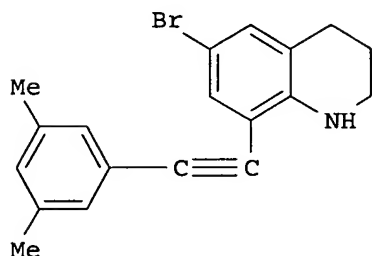
STEREO ATTRIBUTES: NONE  
 L11 18 SEA FILE=REGISTRY SUB=L9 SSS FUL L10  
 L12 7 SEA FILE=HCAPLUS ABB=ON PLU=ON L11  
 L15 43 SEA FILE=HCAPLUS ABB=ON PLU=ON ("EMIG P"/AU OR "EMIG  
 PETER"/AU)  
 L16 41 SEA FILE=HCAPLUS ABB=ON PLU=ON L15 NOT L12

=>

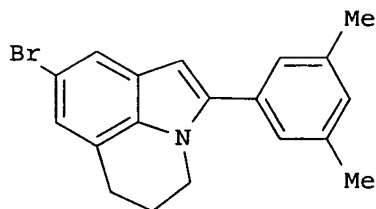
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L16 ANSWER 1 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:348098 HCAPLUS  
 DOCUMENT NUMBER: 143:26477  
 TITLE: Palladium(II)-catalyzed heterocyclization of  
 8-arylethynyl-1,2,3,4-tetrahydroquinolines: A facile  
 route to 2-aryl-5,6-dihydro-4H-pyrrolo[3,2,1-  
 ij]quinoline derivatives  
 AUTHOR(S): Marchand, Pascal; Puget, Alain; Le Baut, Guillaume;  
 Emig, Peter; Czech, Michael; Guenther, Eckhard  
 CORPORATE SOURCE: Laboratoires de Chimie Organique et de Chimie  
 Therapeutique, UPRES EA 1155, Faculte de Pharmacie,  
 Nantes, F-44035, Fr.  
 SOURCE: Tetrahedron (2005), 61(16), 4035-4041  
 CODEN: TETRAB; ISSN: 0040-4020  
 PUBLISHER: Elsevier B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



I

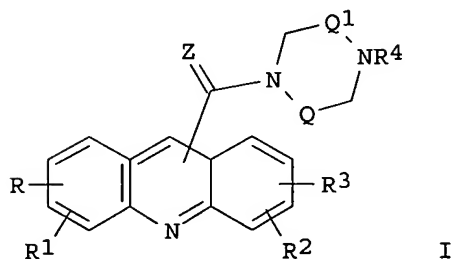


II

AB Dihydropyrroloquinolines have been synthesized reacting  
 8-arylethynyl-1,2,3,4-tetrahydroquinolines in the presence of  
 palladium(II) chloride catalyst. Heteroannulation has been achieved in  
 good yields and tolerates substituents on the tetrahydroquinoline,  
 including bromo, cyano, and ester. E.g., PdCl<sub>2</sub> catalyzed the  
 heterocyclization of 8-arylethynyl-1,2,3,4-tetrahydroquinoline I to give  
 2-aryl-5,6-dihydro-4H-pyrrolo[3,2,1-ij]quinoline II.  
 REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 2 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:74111 HCAPLUS

PATENT NO.				KIND	DATE	APPLICATION NO.				DATE						
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WO 2005007643				A1	20050127	WO 2004-EP7020				20040629						
W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
	CN,	CO,	CR,	CU,	CZ,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	GE,
	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,
	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,	NO,
	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	TJ,
	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW		
RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
	AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,
	SI,	SK,	TR,	BF,	BJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,
	SN,	TD,	TG													
DE 10331500				A1	20050224	DE 2003-10331500				20030711						
PRIORITY APPLN. INFO.:						DE 2003-10331500				A 20030711						
OTHER SOURCE(S):				MARPAT	142:176867											
GI																

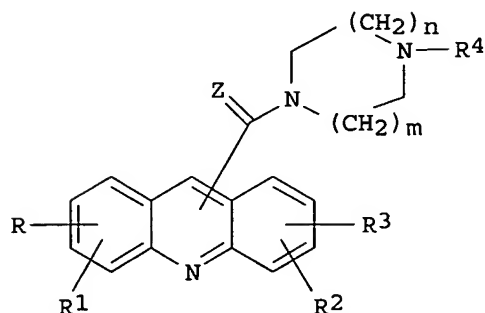


L16 ANSWER 3 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 2005:34599 HCAPLUS  
DOCUMENT NUMBER: 142:134620  
TITLE: Preparation of acridine derivatives as antitumor agents  
INVENTOR(S): Gerlach, Matthias; **Emig, Peter**; Paulini,

Klaus; Czech, Michael; Schuster, Tilman; Gunther, Eckhard  
 PATENT ASSIGNEE(S): Germany  
 SOURCE: U.S. Pat. Appl. Publ., 21 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005009809	A1	20050113	US 2004-879280	20040629
PRIORITY APPLN. INFO.:			US 2003-486525P	P 20030711
OTHER SOURCE(S):	MARPAT 142:134620			

GI



I

AB The invention relates to (heterocyclylcarbonyl)acridine derivs. of the formula (I) [Z = O, S; n, m = 0-4; R, R1, R2, R3 may optionally be attached to the heteroarom. carbon atoms C1 to C9 of the acridine, are identical or different and independently of one another are H, HO or OR5, but the radicals R, R1, R2 and R3 are not simultaneously H; R4 = C6-14 aryl, C6-14 aryl-C1-4 alkyl, C2-10 heteroaryl or C2-10 heteroaryl-C1-4 alkyl containing one or more heteroatoms selected from the group consisting of N, O and S, where the C1-4 alkyl radical may be unsubstituted or mono or polysubstituted; or, if R, R1, R2, R3 may optionally be attached to the heteroarom. carbon atoms C1 to C9 of the acridine, are identical or different and independently of one another and are H, straight-chain or branched C1-8 alkyl, C3-7 cycloalkyl, straight-chain or branched C1-8 alkylcarbonyl, HO, straight-chain or branched C1-8 alkoxy, halogen, straight-chain or branched aryl-C1-8 alkoxy, trityloxy, trimethylsilyloxy, amino, mono(C1-4 alkyl)amino, di(C1-4 alkyl)amino, (C2-5 cycloalkyl)amino, morpholino, etc.; R5 = -SO2-X1 (where X1 = NMe2, hydroxy, alkoxy, etc.), C(O)-X2 (where X2 = (un)substituted alkyl, cycloalkyl, heterocyclyl, aryl, or heteroaryl, etc.), etc.] or physiol. acceptable salts thereof. These compds. are useful for treating benign and malignant tumors in humans and mammals. Thus, 6.66 g (11.06 mmol) polymer-bound N-benzyl-N-cyclohexylcarbodiimide (1.66 mmol/g) was added to a solution of 1.8 g (7.05 mmol) 1,3-dihydroxyacridine-9-carboxylic acid in 40 mL DMF. The mixture was heated at 60° and allowed to react for 30 min, treated with 1.03 g (5.64 mmol) 1-(6-methyl-2-pyridinyl)piperazine, and allowed to react for a further 4 h to give, after workup and silica gel chromatog., 2.3 g (1,3-dihydroxyacridin-9-yl) [4-(6-methylpyridin-2-yl)piperazin-1-yl]methanone (74.8%). The compds. I inhibited the proliferation of human tumor cell lines such as human cervical carcinoma cell line KB/Hela,

ovarian adenocarcinoma cell line SKOV3, human glioblastoma cell line SF-268, and lung carcinoma cell line NCI-H460 with EC50 of 0.007-0.293 µg/mL. Six compds. I were also tested for inhibiting the polymerization of tubulin and exhibited EC50 of 1.08-4.82.

L16 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:1080885 HCAPLUS

DOCUMENT NUMBER: 142:56172

TITLE: Preparation of 1-(4-chlorobenzyl)indoles as tubulin polymerization inhibitors with apoptosis inducing activity

INVENTOR(S): Gerlach, Matthias; Schuster, Tilmann; ~~Emig~~, Peter; Schmidt, Peter; Bassner, Silke; Guenther, Eckhard

PATENT ASSIGNEE(S): Zentaris G.m.b.H., Germany

SOURCE: PCT Int. Appl., 50 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

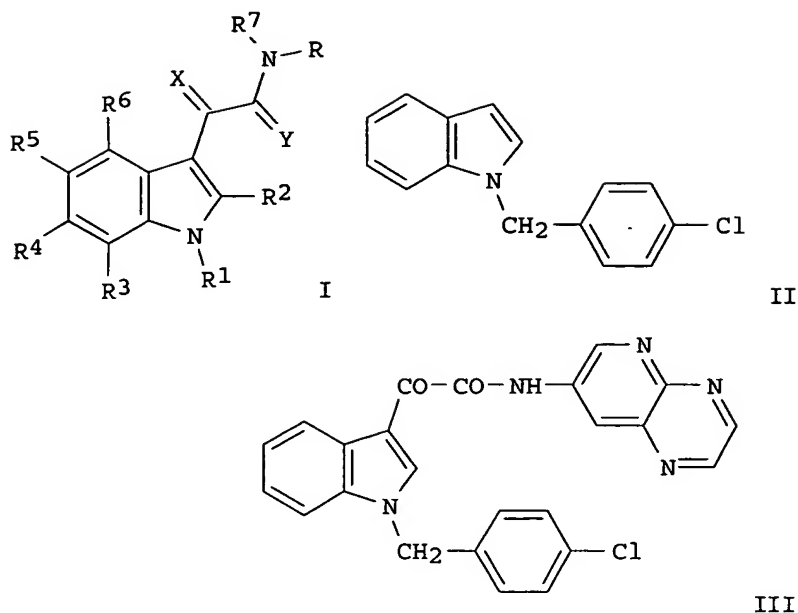
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004108702	A1	20041216	WO 2004-EP5593	20040525
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1484329	A1	20041208	EP 2003-12868	20030606
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
EP 1595878	A1	20051116	EP 2004-11598	20040515
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR			
CA 2526663	AA	20041216	CA 2004-2526663	20040525
PRIORITY APPLN. INFO.:			US 2003-476277P	P 20030605
			EP 2003-12868	A 20030606
			EP 2004-11598	A 20040515
			WO 2004-EP5593	W 20040525

GI



AB Title compounds I [R = (un)substituted heterocycle containing N, O, S heteroatoms; R1 = (un)substituted alkyl-aryl; R2 = H, (un)substituted alkyl; R3, R4, R5, R6 = H, (un)substituted alkyl, cycloalkyl, etc.; R7 = alkylcarbonyl, alkoxy carbonyl; X, Y = S, O] and their pharmaceutically acceptable salts were prepared. For example, oxalyl chloride acylation of chlorobenzylindole II, i.e., prepared from indole and 4-chlorobenzyl chloride, followed by pyrido[2,3-b]pyrazin-7-amine amidation afforded claimed chlorobenzylindole III in 68% yield. In human tubulin polymerization inhibition assays, 4-examples of compds. I exhibited EC50 values ranging from 0.71-1.26  $\mu\text{g/mL}$ , i.e., the EC50 value of chlorobenzylindole III was 0.71  $\mu\text{g/mL}$ . Compds. I are claimed to be useful as antitumor agents.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 5 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:1054280 HCAPLUS

DOCUMENT NUMBER: 142:38145

TITLE: Preparation of 1-(4-chlorobenzyl)indoles as tubulin polymerization inhibitors with apoptosis inducing activity

INVENTOR(S): Emig, Peter; Gerlach, Matthias; Paulini, Klaus; Czech, Michael; Schuster, Tilmann; Schmidt, Peter; Baasner, Silke; Guenther, Eckhard

PATENT ASSIGNEE(S): Zentaris G.m.b.H., Germany

SOURCE: Eur. Pat. Appl., 22 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

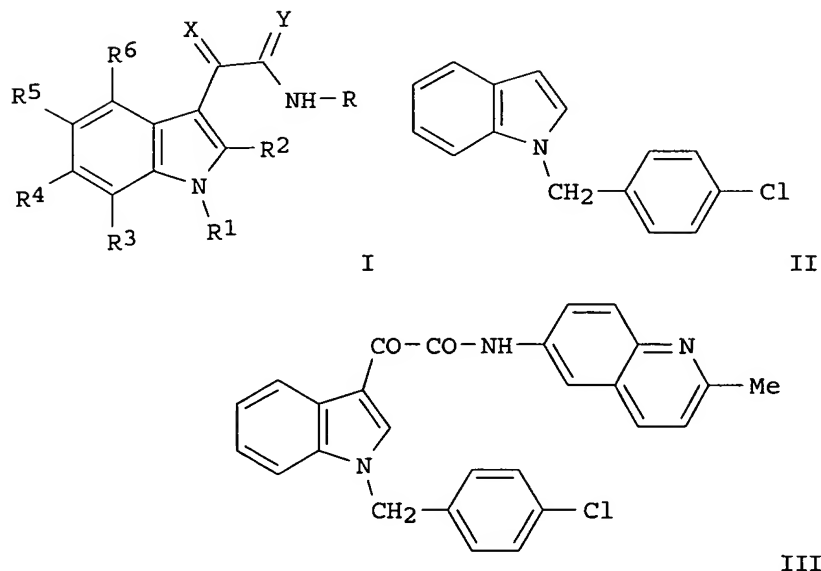
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 1484329 A1 20041208 EP 2003-12868 20030606  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK  
 CA 2526663 AA 20041216 CA 2004-2526663 20040525  
 WO 2004108702 A1 20041216 WO 2004-EP5593 20040525  
 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,  
 CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,  
 GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,  
 LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO,  
 NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,  
 TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,  
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,  
 EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,  
 SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,  
 SN, TD, TG  
 US 2004266762 A1 20041230 US 2004-858751 20040602  
 PRIORITY APPLN. INFO.: US 2003-476277P P 20030605  
 EP 2003-12868 A 20030606  
 US 2003-476794P P 20030606  
 EP 2004-11598 A 20040515  
 US 2004-572025P P 20040517  
 WO 2004-EP5593 W 20040525

GI



AB Title compounds I [R = (un)substituted quinolyl, pyridopyrazinyl, indazolyl; R1 = alkyl-aryl; R2 = H; R3, R4, R5, R6 = H, (un)substituted alkyl, cycloalkyl, etc.; X, Y = S, O] and their pharmaceutically acceptable salts were prepared. For example, oxalyl chloride acylation of chlorobenzylindole II, i.e., prepared from indole and 4-chlorobenzyl chloride, followed by 6-amino-2-methylquinoline amidation afforded claimed chlorobenzylindole III in 77% yield. In human tubulin polymerization inhibition assays, 6-examples of compds. I exhibited EC50 values ranging from 0.71-1.27  $\mu\text{g/mL}$ , i.e., the EC50 value of chlorobenzylindole III



was 1.16 µg/mL. Compds. I are claimed to be useful as antitumor agents.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 6 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:20666 HCAPLUS

DOCUMENT NUMBER: 140:77166

TITLE: Preparation of arylcarbonylpiperazines and heteroarylcarbonylpiperazines for treating benign and malignant tumor diseases

INVENTOR(S): Emig, Peter; Gerlach, Matthias; Polymeropoulos, Emmanuel; Mueller, Gilbert; Schmidt, Peter; Baasner, Silke; Guenther, Eckhard

PATENT ASSIGNEE(S): Zentaris GmbH, Germany

SOURCE: PCT Int. Appl., 45 pp.

CODEN: PIXXD2

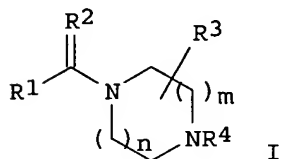
DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004002965	A1	20040108	WO 2003-EP6555	20030620
W: AU, BR, BY, CA, CN, CO, GE, HR, HU, ID, IL, IN, IS, JP, KR, KZ, LT, LV, MK, MX, NO, NZ, PH, PL, RO, RU, SG, UA, UZ, YU, ZA				
RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
AU 2003246571	A1	20040119	AU 2003-246571	20030620
EP 1517898	A1	20050330	EP 2003-761482	20030620
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003012294	A	20050412	BR 2003-12294	20030620
CN 1665792	A	20050907	CN 2003-815485	20030620
NZ 537916	A	20051125	NZ 2003-537916	20030620
JP 2005538968	T2	20051222	JP 2004-516632	20030620
CA 2433983	AA	20031229	CA 2003-2433983	20030627
US 2004097734	A1	20040520	US 2003-608520	20030627
ZA 2004009610	A	20050418	ZA 2004-9610	20041126
NO 2005000428	A	20050125	NO 2005-428	20050125
PRIORITY APPLN. INFO.:			US 2002-393027P	P 20020629
			WO 2003-EP6555	W 20030620
OTHER SOURCE(S):			MARPAT 140:77166	
GI				



AB Title compds. [I; R1 = (substituted) fluoren-9-one, isoxazolyl, cinnolinyl, isothiazolyl, isoquinolinyl, 9H-fluorenyl, 9H-xanthenyl, 1H-pyrazolyl; R2 = O, S; R3 = H, (substituted) alkyl, halo, CO2H, CONH2;

R4 = (substituted) (hetero)aryl, alkylaryl, alkylhetaryl; m, n = 0-3], were prepared Thus, 9-fluorenone-4-carbonyl chloride in DMF was successively treated with N-methylmorpholine, 1-(3,5-dimethoxyphenyl)piperazine, and 1-benzotriazolyltripyrrolidinophosphonium hexafluorophosphate followed by stirring for 12 h at room temperature to give 79,3% 4-[4-(3,5-dimethoxyphenyl)piperazine-1-carbonyl]fluoren-9-one. The latter inhibited proliferation in XTT cytotoxicity test in human tumor cells with EC50 = 0,2-0,555 µg/mL.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 7 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:107333 HCAPLUS

DOCUMENT NUMBER: 136:167288

TITLE: Preparation of N-(6-quinolinyl)-3-indolylglyoxylamides as antitumor agents

INVENTOR(S): Emig, Peter; Bacher, Gerald; Reichert, Dietmar; Baasner, Silke; Aue, Beate; Nickel, Bernd; Guenther, Eckhard

PATENT ASSIGNEE(S): Zentaris A.-G., Germany

SOURCE: PCT Int. Appl., 44 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

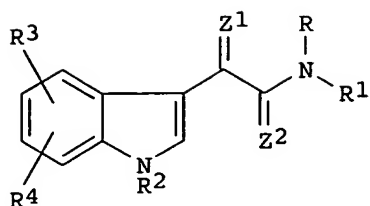
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002010152	A2	20020207	WO 2001-EP8644	20010726
WO 2002010152	A3	20020801		
W:	AU, BG, BR, BY, CN, CO, CZ, EE, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LT, LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, UZ, YU, ZA, AM, AZ, MD, TJ, TM			
RW:	AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR			
DE 10037310	A1	20020207	DE 2000-10037310	20000728
US 2003100597	A1	20030529	US 2001-910140	20010720
CA 2354210	AA	20020128	CA 2001-2354210	20010726
EP 1309585	A2	20030514	EP 2001-969522	20010726
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, TR			
BR 2001012807	A	20030701	BR 2001-12807	20010726
JP 2004505075	T2	20040219	JP 2002-515883	20010726
NZ 524404	A	20040827	NZ 2001-524404	20010726
RU 2270196	C2	20060220	RU 2003-105891	20010726
ZA 2003000584	A	20030718	ZA 2003-584	20030122
NO 2003000382	A	20030220	NO 2003-382	20030124
BG 107560	A	20031031	BG 2003-107560	20030214
PRIORITY APPLN. INFO.:			DE 2000-10037310	A 20000728
			WO 2001-EP8644	W 20010726

OTHER SOURCE(S): MARPAT 136:167288

GI



I

AB Title compds. [I; R = H, (substituted) alkyl, alkoxyalkyl, arylalkyloxycarbonyl, etc.; R1 = (substituted) (un)saturated and aromatic heterocyclyl especially (substituted) 2-, 3-, 4- and 8-quinolinyl and 2-, 3-, 4-quinolinylmethyl; R2 = H, (substituted) phenylalkyl, etc.; R3, R4 = H, OH, alkyl, cycloalkyl, alkylcarbonyl, alkoxy, etc.; Z1 = O, S, H, OH; Z2 = O, S] and salts thereof were prepared Thus, (COCl)<sub>2</sub> in ether was dropwise treated with 1-(4-chlorobenzyl)indole (preparation given) in ether under N<sub>2</sub>-atmosphere followed by reflux for 2 h and removal of solvent. The resulting reaction mixture in THF was dropwise treated with 6-amino-2-methylquinoline in THF followed by reflux for 4 h and then the reaction mixture was kept overnight at room temperature to give 77.3% N-(2-methyl-6-quinolinyl)-[1-(4-chlorobenzyl)indol-3-yl]glyoxylamide. The latter induced growth inhibition of e.g. human cervical carcinoma cell lines KB/HeLa with IC<sub>50</sub> = 0.17  $\mu$ M in a proliferation test.

L16 ANSWER 8 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:90014 HCAPLUS

DOCUMENT NUMBER: 136:134791

TITLE: Preparation of acridinylcarbonylpiperazines related compounds as anticancer drugs.

INVENTOR(S): **Emig, Peter**; Guenther, Eckhard; Baasner, Silke; Bacher, Gerald; Beckers, Thomas; Aue, Beate

PATENT ASSIGNEE(S): Zentaris A.-G., Germany

SOURCE: PCT Int. Appl., 46 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

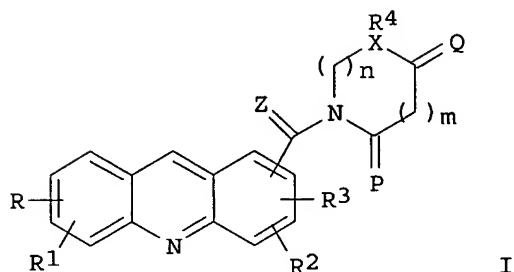
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008194	A1	20020131	WO 2001-EP8263	20010718
WO 2002008194	C1	20030508		
W: AU, BG, BR, BY, CN, CO, CZ, EE, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LT, LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, UZ, YU, ZA				
RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
DE 10035927	A1	20020307	DE 2000-10035927	20000721
EP 1301485	A1	20030416	EP 2001-969410	20010718
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, TR				
BR 2001012591	A	20030722	BR 2001-12591	20010718
JP 2004504382	T2	20040212	JP 2002-514101	20010718
NZ 524155	A	20050429	NZ 2001-524155	20010718
RU 2267488	C2	20060110	RU 2003-105283	20010718
CA 2353360	AA	20020121	CA 2001-2353360	20010720
US 2002132821	A1	20020919	US 2001-910142	20010720

US 6706722 B2 20040316  
 ZA 2002010411 A 20030226 ZA 2002-10411 20021223  
 NO 2003000301 A 20030311 NO 2003-301 20030120  
 BG 107507 A 20030930 BG 2003-107507 20030130  
 PRIORITY APPLN. INFO.: DE 2000-10035927 A 20000721  
 WO 2001-EP8263 W 20010718  
 OTHER SOURCE(S): MARPAT 136:134791  
 GI



AB Title compds. [I; R-R3 = H, alkyl, cycloalkyl, alkylcarbonyl, alkoxy, halo, aralkoxy, NO2, amino, alkoxy-carbonylamino, cyano, cyanoalkyl, CO2H, alkoxy-carbonyl, CF3, etc.; Z = O, S; P, Q = O, H2; X = N, CR5; R5 = H, alkyl; m, n = 0-3; R4 = (substituted) (unsatd.) alkyl, aryl, aralkyl, etc.], were prepared. Thus, acridine-9-carboxylic acid in DMF was treated with N-methylmorpholine, Py-BOP, (1-benzotriazolyltripyrrolidinophosphonium hexafluorophosphate), and 1-(3,5-dimethoxyphenyl)piperazine in DMF. The mixture was stirred 12 h to give 84.2% 1-(3,5-dimethoxyphenyl)-4-(9-acridinylcarbonyl)piperazine. The latter inhibited KB/HeLa cell growth with IC50 <0.0003 µg/mL.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 9 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:90012 HCAPLUS

DOCUMENT NUMBER: 136:134790

TITLE: Preparation of quinolylcarbonylpiperazines and related compounds for treatment of tumors.

INVENTOR(S): Emig, Peter; Guenther, Eckhard; Schmidt, Juergen; Nickel, Bernd; Kutscher, Bernhard

PATENT ASSIGNEE(S): Zentaris A.-G., Germany

SOURCE: PCT Int. Appl., 44 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

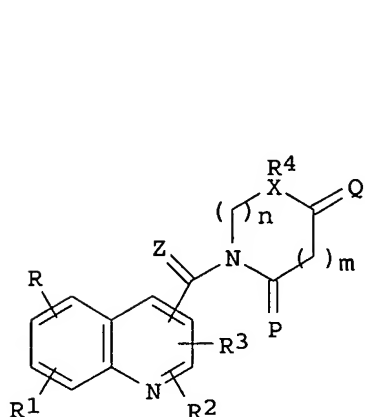
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008192	A1	20020131	WO 2001-EP8261	20010718
W: AU, BG, BR, BY, CN, CO, CZ, EE, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LT, LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, UZ, YU, ZA, AM, AZ, MD, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
DE 10035928	A1	20020307	DE 2000-10035928	20000721

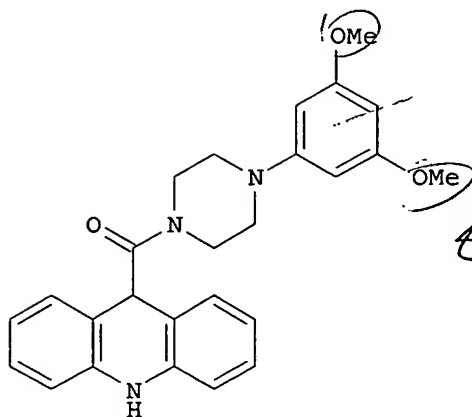
EP 1305290	A1	20030502	EP 2001-957978	20010718
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001012589	A	20030520	BR 2001-12589	20010718
JP 2004504381	T2	20040212	JP 2002-514099	20010718
NZ 524154	A	20050225	NZ 2001-524154	20010718
RU 2265602	C2	20051210	RU 2003-105278	20010718
CA 2353369	AA	20020121	CA 2001-2353369	20010720
US 2002103214	A1	20020801	US 2001-910141	20010720
US 6890926	B2	20050510		
ZA 2002010180	A	20030212	ZA 2002-10180	20021217
NO 2003000298	A	20030120	NO 2003-298	20030120
BG 107508	A	20030930	BG 2003-107508	20030130
US 2004097530	A1	20040520	US 2003-713859	20031114
US 2004132747	A1	20040708	US 2003-741310	20031219
US 6936615	B2	20050830		
US 2005176744	A1	20050811	US 2005-105622	20050414
US 2005245523	A1	20051103	US 2005-152599	20050614
PRIORITY APPLN. INFO.:			DE 2000-10035928	A 20000721
			WO 2001-EP8261	W 20010718
			US 2001-910141	A3 20010720
			US 2003-741310	A3 20031219

OTHER SOURCE(S):  
GI

MARPAT 136:134790



I



II

AB Title compds. [I; R-R<sub>3</sub> = H, alkyl, cycloalkyl, alkylcarbonyl, alkoxy, halo, aralkoxy, NO<sub>2</sub>, amino, cyano, CO<sub>2</sub>H, CF<sub>3</sub>, etc.; RR<sub>1</sub>, R<sub>2</sub>R<sub>3</sub> = atoms to form condensed 6-membered aromatic rings; Z = O, S; X = N, CR<sub>5</sub>; R<sub>5</sub> = H, alkyl; R<sub>4</sub> = (substituted) (unsatd.) alkyl, aryl, aralkyl, etc.; P, Q = O, H<sub>2</sub>; m, n = 0-3], were prepared. Thus, quinoline-4-carboxylic acid in DMF was treated with N-methylmorpholine, Py-BOP (1-benzotriazolyltripyrrolidinophosphoniumhexafluorophosphate), and 1-(3,5-dimethoxyphenyl)piperazine in DMF. The mixture was stirred 12 h to give 78.3% 1-(3,5-dimethoxyphenyl)-4-(4-quinolylcarbonyl)piperazine. Title compound (II) (D-43411) showed antiproliferative activity with IC<sub>50</sub> <0.0003 µg/mL against SKOV-3 tumor cells.

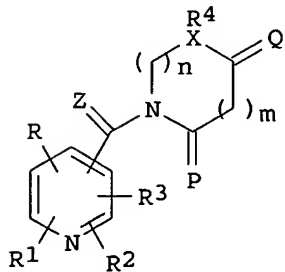
REFERENCE COUNT:

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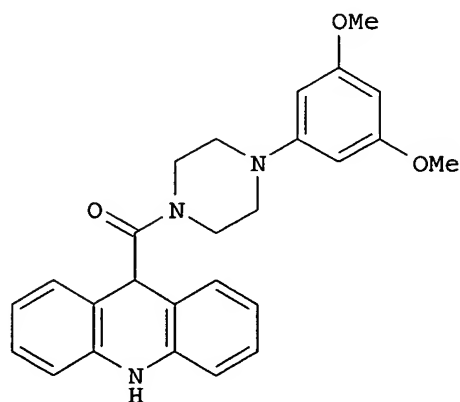
THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2002:90010 HCAPLUS  
 DOCUMENT NUMBER: 136:134789  
 TITLE: Preparation of pyridylcarbonylpiperazines and related compounds as anticancer drugs.  
 INVENTOR(S): **Emig, Peter**; Guenther, Eckhard; Schmidt, Juergen; Kutscher, Bernhard; Nickel, Bernd; Storch, Anita  
 PATENT ASSIGNEE(S): Zentaris A.-G., Germany  
 SOURCE: PCT Int. Appl., 40 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008190	A2	20020131	WO 2001-EP8262	20010718
WO 2002008190	A3	20020801		
W: AU, BG, BR, BY, CN, CO, CZ, EE, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LT, LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, UZ, YU, ZA, AM, AZ, MD, TJ, TM RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
DE 10035908	A1	20020307	DE 2000-10035908	20000721
EP 1305289	A2	20030502	EP 2001-960509	20010718
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, TR				
BR 2001012711	A	20030520	BR 2001-12711	20010718
JP 2004516243	T2	20040603	JP 2002-514097	20010718
NZ 524156	A	20051028	NZ 2001-524156	20010718
CA 2353353	AA	20020121	CA 2001-2353353	20010720
US 2002111354	A1	20020815	US 2001-910139	20010720
US 6638935	B2	20031028		
ZA 2003000545	A	20030212	ZA 2003-545	20020121
NO 2003000302	A	20030207	NO 2003-302	20030120
BG 107506	A	20030930	BG 2003-107506	20030130
PRIORITY APPLN. INFO.:			DE 2000-10035908	A 20000721
			WO 2001-EP8262	W 20010718
OTHER SOURCE(S):	MARPAT 136:134789			
GI				



I



II

AB Title compds. [I; R-R3 = H, alkyl, cycloalkyl, alkylcarbonyl, alkoxy, halo, aralkoxy, NO2, amino, cyano, CO2H, alkoxycarbonyl, CF3, etc.; RR1, R2R3 = atoms to form fused 6-membered aromatic rings; Z = O, S; P, Q = O, H2; X = N, CR5; m, n = 0-3; R4 = (substituted) (unsatd.) alkyl, aryl, aralkyl, etc.], were prepared. Thus, pyridine-4-carboxylic acid in DMF was treated with N-methylmorpholine, Py-BOP (1-benzotriazolyltripyrrolidinophosphonium hexafluorophosphate), 1-(3,5-dimethoxyphenyl)piperazine followed by stirring for 24 h to give 82.3% 1-(3,5-dimethoxyphenyl)-4-(4-pyridylcarbonyl)piperazine. Title compound (II) inhibited L1210 tumor cells with IC50<0.0003 µg/mL.

L16 ANSWER 11 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:915607 HCAPLUS  
 DOCUMENT NUMBER: 136:193482  
 TITLE: New small-molecule tubulin inhibitors  
 AUTHOR(S): Bacher, G.; Beckers, T.; Emig, P.; Klenner, T.; Kutschert, B.; Nickel, B.  
 CORPORATE SOURCE: IUPAC Commission, Research & Development Oncology, ASTA Medica AG, Frankfurt, 60314, Germany  
 SOURCE: Pure and Applied Chemistry (2001), 73(9), 1459-1464  
 CODEN: PACHAS; ISSN: 0033-4545  
 PUBLISHER: International Union of Pure and Applied Chemistry  
 DOCUMENT TYPE: Journal; General Review  
 LANGUAGE: English

AB A review. The variety of biol. agents directed toward the tubulin system exceeds those acting on DNA, making it an important target for cancer chemotherapy. However, the complicated chemical structures and restricted access to the natural resources, in combination with the development of drug resistance, limit the first generation of natural products. Considerable efforts in the search and synthesis of new synthetic compds., such as small mol. tubulin inhibitors, gave access to novel potential/promising drugs. Among these substances, two series of novel, easily accessible indole classes were identified as tubulin-destabilizing agents. Owing to the synthetic nature, potent in vitro and in vivo antitumoral activity, and efficacy against multidrug-resistant (MDR) tumors, D-24851 and D-64131 have significant potential in cancer treatment.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 12 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:858552 HCAPLUS  
 DOCUMENT NUMBER: 136:247463  
 TITLE: Synthesis and pharmacological evaluation of (indol-3-yl)alkylamides as potent analgesic agents  
 AUTHOR(S): Fouchard, Fabienne; Marchand, Pascal; Le Baut, Guillaume; Emig, Peter; Nickel, Bernd  
 CORPORATE SOURCE: Laboratoires de Chimie Organique et de Chimie Therapeutique, Faculte de Pharmacie, Nantes, 44035, Fr.  
 SOURCE: Arzneimittelforschung (2001), 51(10), 814-824  
 CODEN: ARZNAD; ISSN: 0004-4172  
 PUBLISHER: Editio Cantor Verlag  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 136:247463

AB A series of (indol-3-yl)alkylamides was synthesized and evaluated for analgesic activity. Two N-(pyridin-4-yl)acetamides, bearing benzyl or

4-fluorobenzyl moieties in 1-position of indole ring, exhibited promising analgesic properties (ED<sub>50</sub> = 8.1 and 11 mg/kg p.o., resp.). The two test compds. were tested for their anti-inflammatory activity by carrageenin-induced edema in rat paw test. 4-Fluorobenzyl derivative whose ID<sub>50</sub> was 0.085 ± 0.021 mmol/kg was selected as a lead compound for further pharmacomodulation.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 13 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:790429 HCAPLUS

DOCUMENT NUMBER: 136:200078

TITLE: Synthesis and characterization of the biologically active 2-[1-(4-chlorobenzyl)-1H-indol-3-yl]-2-oxo-N-pyridin-4-yl acetamide

AUTHOR(S): Knaack, Martin; Emig, Peter; Bats, Jan W.;

Kiesel, Michael; Muller, Arndt; Gunther, Eckhard

CORPORATE SOURCE: Infracor GmbH, Hanau, 63457, Germany

SOURCE: European Journal of Organic Chemistry (2001), (20), 3843-3847

CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:200078

AB The spectroscopic characterization of the new potent tubulin inhibitor 2-[1-(4-chlorobenzyl)-1H-indol-3-yl]-2-oxo-N-pyridin-4-yl acetamide (D-24851), which is under preclin. development, is described. The synthesis was optimized and follows a straightforward route from the unsubstituted indole via 1-(4-chlorobenzyl)indole and 1-[(4-chlorophenyl)methyl]- $\alpha$ -oxo-N-4-pyridinyl-1H-indole-3-acetyl chloride to the target compound, D-24851. The structure was assigned by sophisticated NMR expts., for example a 1,1-ADEQUATE experiment, and X-ray crystallog.

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 14 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:467995 HCAPLUS

DOCUMENT NUMBER: 135:46111

TITLE: Preparation of N-(pyridin-4-yl) [1-(4-aminobenzyl)indol-3-yl]glyoxylamides as antitumor agents

INVENTOR(S): Guenther, Eckhard; Emig, Peter; Reichert, Dietmar; Le Baut, Guillaume; Nickel, Bernd; Bacher, Gerald

PATENT ASSIGNEE(S): Asta Medica A.-G., Germany

SOURCE: Ger. Offen., 10 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

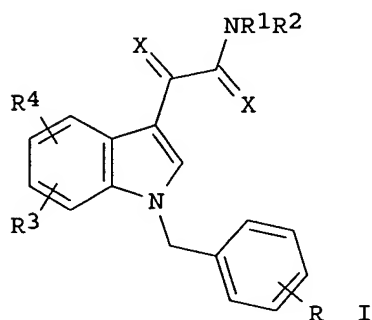
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19962300	A1	20010628	DE 1999-19962300	19991223
US 2001014690	A1	20010816	US 2000-736431	20001215
US 6432987	B2	20020813		
CA 2395259	AA	20010705	CA 2000-2395259	20001219



WO 2001047913                      A2                      20010705                      WO 2000-EP12947                      20001219  
W: AT, AU, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE,  
HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LT, LU, LV, MK, MX, NO,  
NZ, PL, PT, RO, RU, SE, SG, SI, SK, TR, UA, UZ, YU, ZA, AM, AZ,  
MD, TJ, TM  
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,  
PT, SE, TR  
BR 2000016712                      A                      20020903                      BR 2000-16712                      20001219  
EP 1240157                      A2                      20020918                      EP 2000-983349                      20001219  
EP 1240157                      B1                      20040211  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, TR  
JP 2003519137                      T2                      20030617                      JP 2001-549383                      20001219  
AT 259364                      E                      20040215                      AT 2000-983349                      20001219  
AU 772745                      B2                      20040506                      AU 2001-20119                      20001219  
PT 1240157                      T                      20040630                      PT 2000-983349                      20001219  
NZ 519977                      A                      20040827                      NZ 2000-519977                      20001219  
ES 2215768                      T3                      20041016                      ES 2000-983349                      20001219  
NZ 533731                      A                      20050324                      NZ 2000-533731                      20001219  
RU 2266280                      C2                      20051220                      RU 2002-120462                      20001219  
ZA 2002004896                      A                      20021220                      ZA 2002-4896                      20020619  
NO 2002003039                      A                      20020809                      NO 2002-3039                      20020621  
BG 106924                      A                      20030430                      BG 2002-106924                      20020716  
PRIORITY APPLN. INFO.:                      DE 1999-19962300                      A                      19991223  
OTHER SOURCE(S):                      MARPAT 135:46111                      WO 2000-EP12947                      W                      20001219  
GI



AB Title compds. [I; R1 = H, (substituted) alkyl, benzyloxycarbonyl, t-butoxycarbonyl, OAc; R2 = (substituted) Ph, pyridinyl, pyrimidinyl, etc.; or R1R2 = (substituted) (homo)piperazinyl; R3, R4 = H, alkyl, cycloalkyl, alkanoyl, alkoxy, halo, PhCH2O, NO2, amino, etc.; R = NO2, amino, (di)alkylamino, cycloalkylamino, phenylalkylamino, (hetero)aroylamino, etc.; X = O, S] were prepared as antitumor agents (no data). Thus, (COCl)<sub>2</sub> in Et<sub>2</sub>O at 0° was treated dropwise with indole in Et<sub>2</sub>O and refluxed for 3 h followed by dropwise addition of 4-aminopyridine in THF at 5° and reflux over night to give 43.3% N-(pyridin-4-yl) (indol-3-yl)glyoxylamide. The product was treated with 4-nitrobenzyl chloride to give 64% N-(pyridin-4-yl) [1-(4-nitrobenzyl)indol-3-yl]glyoxylamide (D-68836). The latter was subjected to catalytic hydrogenation to give 94% N-(pyridin-4-yl) [1-(4-aminobenzyl)indol-3-yl]glyoxylamide (D-68838). D-68838 was said to inhibit polymerization of tubulin.

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 15 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:247170 HCAPLUS

DOCUMENT NUMBER: 134:261240

TITLE: Indolyl-3-glyoxylic acid derivatives comprising therapeutically valuable properties

INVENTOR(S): Nickel, Bernd; Klenner, Thomas; Bacher, Gerald; Beckers, Thomas; ~~Emig, Peter~~; Engel, Juergen; Bruyneel, Erik; Kamp, Guenter; Peters, Kirsten

PATENT ASSIGNEE(S): Asta Medica Ag, Germany

SOURCE: PCT Int. Appl., 30 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001022954	A2	20010405	WO 2000-EP9390	20000926
WO 2001022954	A3	20020328		
W: AU, BG, BR, BY, CA, CN, CZ, DZ, EE, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LT, LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US, UZ, YU, ZA, AM, AZ, MD, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
DE 19946301	A1	20010419	DE 1999-19946301	19990928
US 2003114511	A1	20030619	US 2000-492531	20000127
US 6693119	B2	20040217		
CA 2386069	AA	20010405	CA 2000-2386069	20000926
EP 1218006	A2	20020703	EP 2000-967789	20000926
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003510274	T2	20030318	JP 2001-526166	20000926
EE 200200169	A	20030415	EE 2002-169	20000926
BR 2000014378	A	20030729	BR 2000-14378	20000926
NZ 517988	A	20041029	NZ 2000-517988	20000926
AU 783436	B2	20051027	AU 2000-77829	20000926
NO 2002001367	A	20020522	NO 2002-1367	20020319
ZA 2002002556	A	20030704	ZA 2002-2556	20020402
BG 106639	A	20021229	BG 2002-106639	20020423
US 2004171668	A1	20040902	US 2003-686809	20031017
PRIORITY APPLN. INFO.:			DE 1999-19946301	A 19990928
			DE 1998-19814838	A 19980402
			US 1999-285058	A2 19990402
			US 2000-492531	A1 20000127
			WO 2000-EP9390	W 20000926

OTHER SOURCE(S): MARPAT 134:261240

AB The invention relates to the use of N-substituted indol-3- glyoxylamides of for treating tumors, in particular, in cases of drug resistance and metastatic carcinoma, and as angiogenesis inhibitors having distinctly fewer side effects, in particular, distinctly lower neurotoxicity. The invention also relates to medicaments containing the inventive compds.

L16 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:58000 HCAPLUS

DOCUMENT NUMBER: 134:290069

TITLE: D-24851, a novel synthetic microtubule inhibitor, exerts curative antitumoral activity in vivo, shows

efficacy toward multidrug-resistant tumor cells, and lacks neurotoxicity

AUTHOR(S): Bacher, Gerald; Nickel, Bernd; **Emig, Peter**; Vanhoefer, Udo; Seeber, Siegfried; Shandra, Alexei; Klenner, Thomas; Beckers, Thomas

CORPORATE SOURCE: Department of Cancer Research, ASTA Medica AG, Frankfurt am Main, 60314, Germany

SOURCE: Cancer Research (2001), 61(1), 392-399  
CODEN: CNREA8; ISSN: 0008-5472

PUBLISHER: American Association for Cancer Research

DOCUMENT TYPE: Journal

LANGUAGE: English

AB N-(pyridin-4-yl)-[1-(4-chlorobenzyl)indol-3-yl]glyoxylamide (D-24851) is a novel synthetic compound that was identified in a cell-based screening assay to discover cytotoxic drugs. D-24851 destabilizes microtubules and blocks cell cycle transition specifically at G2-M phase. The binding site of D-24851 does not overlap with the tubulin binding sites of known microtubule-destabilizing agents like vincristine or colchicine. In vitro, D-24851 has potent cytotoxic activity toward a panel of established human tumor cell lines including SKOV3 ovarian cancer, U87 glioblastoma, and ASPC-1 pancreatic cancer cells. In vivo, oral D-24851 treatment induced complete tumor regressions (cures) in rats bearing Yoshida AH13 sarcomas. Of importance is that the administration of curative doses of D-24851 to the animals revealed no systemic toxicity in terms of body weight loss and neurotoxicity in contrast to the administration of paclitaxel or vincristine. Interestingly, multidrug-resistant cell lines generated by vincristine-driven selection or transfection with the Mr 170,000 P-glycoprotein encoding cDNA were rendered resistant toward paclitaxel, vincristine, or doxorubicin but not towards D-24851 when compared with the parental cells. Because of its synthetic nature, its oral applicability, its potent in vitro and in vivo antitumoral activity, its efficacy against multidrug-resistant tumors, and the lack of neurotoxicity, D-24851 may have significant potential for the treatment of various malignancies.

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 17 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:659229 HCAPLUS

DOCUMENT NUMBER: 131:271807

TITLE: Preparation of indolyglyoxylamides as antitumor agents

INVENTOR(S): Nickel, Bernd; Szelenyi, Istvan; Schmidt, Jurgen; **Emig, Peter**; Reichert, Dietmar; Gunther, Eckhard; Brune, Kay

PATENT ASSIGNEE(S): Asta Medica A.-G., Germany

SOURCE: PCT Int. Appl., 47 pp.  
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 9951224	A1	19991014	WO 1999-EP1918	19990322
W:	AU, BG, BR, BY, CA, CN, CZ, EE, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LT, LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, UZ, YU, ZA, AM, AZ, MD, TJ, TM			
RW:	AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE			

DE 19814838	A1	19991014	DE 1998-19814838	19980402
DE 19814838	C2	20010118		
CA 2326833	AA	19991014	CA 1999-2326833	19990322
AU 9929349	A1	19991025	AU 1999-29349	19990322
AU 768510	B2	20031218		
BR 9909902	A	20001226	BR 1999-9902	19990322
EP 1071420	A1	20010131	EP 1999-910372	19990322
EP 1071420	B1	20050914		

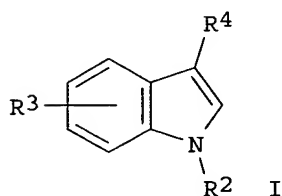
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO

TR 200002853	T2	20010221	TR 2000-200002853	19990322
EE 200000581	A	20020215	EE 2000-581	19990322
EE 4354	B1	20041015		
JP 2002510622	T2	20020409	JP 2000-541995	19990322
NZ 507084	A	20031031	NZ 1999-507084	19990322
AT 304352	E	20050915	AT 1999-910372	19990322
RU 2262339	C2	20051020	RU 2000-128035	19990322
US 6232327	B1	20010515	US 1999-285058	19990402
US 2003114511	A1	20030619	US 2000-492531	20000127
US 6693119	B2	20040217		
NO 2000004916	A	20001201	NO 2000-4916	20000929
HR 2000000643	A1	20010430	HR 2000-643	20001002
BG 104849	A	20010531	BG 2000-104849	20001012
ZA 2000006150	A	20010111	ZA 2000-6150	20001031
US 2003023093	A1	20030130	US 2001-810604	20010319
HK 1036408	A1	20050218	HK 2001-107405	20011024
US 2003195360	A1	20031016	US 2002-309204	20021204
US 2004171668	A1	20040902	US 2003-686809	20031017

PRIORITY APPLN. INFO.:

DE 1998-19814838	A	19980402
WO 1999-EP1918	W	19990322
US 1999-285058	A1	19990402
DE 1999-19946301	A	19990928
US 2000-492531	A1	20000127
US 2001-810604	A1	20010319

OTHER SOURCE(S): MARPAT 131:271807  
GI



AB Title compds. [I; R2 = H or (un)substituted alkyl; R3 = H or 1 or 2 of halo, alkyl, alkoxy, etc.; R4 = C(:X)C(:X)NRR1; R = H, (un)substituted alkyl, CO2CH2Ph, etc.; R1 = (un)substituted Ph, -pyridyl, -pyrimidyl, etc.; RR1 = (CH2CH2)2NR7; R7 = alkyl, Ph, CHPh2, etc.; X = O or S] were prepared. Thus, indole was N-alkylated by 4-FC6H4CH2Cl and the product acylated by (COCl)2 to give, after 4-aminopyridine amidation, I (R2 = CH2C6H4F-4, R3 = H, R4 = COCONHR1, R1 = 4-pyridyl). Data for biol. activity of I were given.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 1999:65867 HCAPLUS  
DOCUMENT NUMBER: 130:223153  
TITLE: New N-(Pyridin-4-yl)-(indol-3-yl)acetamides and Propanamides as Antiallergic Agents  
AUTHOR(S): Menciu, Cecilia; Duflos, Muriel; Fouchard, Fabienne; Le Baut, Guillaume; **Emig, Peter**; Achterrath, Ute; Szelenyi, Istvan; Nickel, Bernd; Schmidt, Juergen; Kutscher, Bernhard; Guenther, Eckhardt  
CORPORATE SOURCE: Department of Organic Chemistry and Medicinal Chemistry, Faculty of Pharmacy, Nantes, 44035, Fr.  
SOURCE: Journal of Medicinal Chemistry (1999), 42(4), 638-648  
CODEN: JMCMAR; ISSN: 0022-2623  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB A series of new N-(pyridin-4-yl)-(indol-3-yl)alkylamides has been prepared in the search of novel antiallergic compds. Synthesis of the desired Et (2-methyindol-3-yl)acetates was achieved by indolization under Fischer conditions; Japp-Klingemann method followed by 2-decarboxylation afforded the Et (indol-3-yl)alkanoates. Amidification was successfully carried out by condensation of the acids or their N-aryl(methyl) derivs. with 4-aminopyridine promoted by 2-chloro-1-methylpyridinium iodide. Efforts to improve the antiallergic potency of the title series by variation of the indole substituents (R1, R2, R) and the length of the alkanoic chain (n = 1, 2, 3) led to the selection of N-(pyridin-4-yl)-[1-(4-fluorobenzyl)indol-3-yl]acetamide (I), out of 41 compds. This amide was 406-fold more potent than astemizole in the ovalbumin-induced histamine release assay, using guinea pig peritoneal mast cells, with an IC50 = 0.016  $\mu$ M. Its inhibitory activity in IL-4 production test from Th-2 cells was identical to that of the reference histamine antagonist (IC50 = 8.0  $\mu$ M) and twice higher in IL-5 assay: IC50 = 1.5 and 3.3  $\mu$ M, resp. In vivo antiallergic activity evaluation confirmed efficiency of I in sensitized guinea pig late phase eosinophilia inhibition, after parenteral and oral administration at 5 and 30 mg/kg, resp. Its efficiency in inhibition of microvascular permeability was assessed in two rhinitis models; ovalbumin and capsaicin-induced rhinorrhea could be prevented after topical application of submicromolar concns. of 45 (IC50 = 0.25 and 0.30  $\mu$ M); and it also exerted significant inhibitory effect in the first test after i.v. and oral administration, with ID50 = 0.005 and 0.46 mg/kg.

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 19 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:46386 HCAPLUS  
DOCUMENT NUMBER: 130:100782  
TITLE: Polymorphism and desolvation of flupirtine maleate  
AUTHOR(S): Landgraf, Karl-Friedrich; Olbrich, Alfred; Pauluhn, Siegfried; **Emig, Peter**; Kutscher, Bernhard; Stange, Hans  
CORPORATE SOURCE: ASTA Medica A.-G., Dresden, Germany  
SOURCE: European Journal of Pharmaceutics and Biopharmaceutics (1998), 46(3), 329-337  
CODEN: EJPBEL; ISSN: 0939-6411  
PUBLISHER: Elsevier Science Ireland Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Crystallizates of the analgesic agent flupirtine maleate (Katadolon; ASTA Medica, Dresden, Germany) obtained from isopropanol are examined by x-ray diffractometry, polarization microscopy and thermoanal. Depending on the crystallizing conditions, the modifications A and B as well as an isopropanol

solvate are observed. The inversion temperature A → B of the enantiotropic modifications is 164° (differential scanning calorimetry (DSC) onset). During thermal desolvation, modification B is formed well below the inversion temperature. In concentrated isopropanol suspensions, the solvate and

modification B are rapidly transformed into modification A. It is shown how phase-pure products consisting of modification A, which is better wettable with water and stable at room temperature, can be obtained.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 20 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:709053 HCAPLUS

DOCUMENT NUMBER: 129:316153

TITLE: Preparation of pure flupirtin maleate and its A crystal modification.

INVENTOR(S): Olbrich, Alfred; **Emig, Peter**; Kutscher, Bernhard; Landgraf, Karl-Friedrich; Pauluhn, Siegfried; Stange, Hans

PATENT ASSIGNEE(S): Asta Medica Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9847872	A1	19981029	WO 1998-EP2118	19980411
W: AU, BR, CA, CN, CZ, HU, IS, JP, NO, PL, RU, SK				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
DE 19716984	A1	19981029	DE 1997-19716984	19970423
AU 9873346	A1	19981113	AU 1998-73346	19980411
EP 977736	A1	20000209	EP 1998-920511	19980411
EP 977736	B1	20030924		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2001523236	T2	20011120	JP 1998-544940	19980411
AT 250579	E	20031015	AT 1998-920511	19980411
PT 977736	T	20040227	PT 1998-920511	19980411
ES 2207832	T3	20040601	ES 1998-920511	19980411
ZA 9803376	A	19980703	ZA 1998-3376	19980422
US 5959115	A	19990928	US 1998-64790	19980423
PRIORITY APPLN. INFO.:			DE 1997-19716984	A 19970423
			WO 1998-EP2118	W 19980411

AB Flupirtin maleate (I) was prepared by hydrogenation of 2-amino-3-nitro-6-(4-fluorobenzylamino)pyridine (II) using Raney Ni, acylation with EtO<sub>2</sub>CCl, and treatment of the resulting flupirtin with maleic acid. Thus, II in Me<sub>2</sub>CHOH was hydrogenated over Raney Ni at 65° and 5 bar H<sub>2</sub>; EtO<sub>2</sub>CCl and Et<sub>3</sub>N were added followed by stirring at 60°, filtration at 50-60° into a solution of maleic acid in H<sub>2</sub>O to precipitate I (89.6% yield). I A crystal modification was obtained by stirring I A and B crystal modification mixture in Me<sub>2</sub>CHOH.

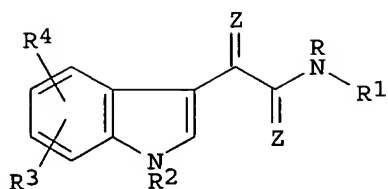
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 21 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:175908 HCAPLUS

DOCUMENT NUMBER: 128:217285  
 TITLE: Preparation of new, N-substituted indole-3-glyoxylamides as antiasthmatics, antiallergic agents and immunosuppressants/immunomodulators  
 INVENTOR(S): Lebaut, Guillaume; Menciu, Cecilia; Kutscher, Bernhard; Emig, Peter; Szelenyi, Stefan; Brune, Kay  
 PATENT ASSIGNEE(S): Asta Medica Aktiengesellschaft, Germany  
 SOURCE: PCT Int. Appl., 40 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9809946	A1	19980312	WO 1997-EP4474	19970816
W: AU, BR, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RU, SG, SK, TR, UA				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
DE 19636150	A1	19980312	DE 1996-19636150	19960906
AU 9740158	A1	19980326	AU 1997-40158	19970816
AU 726521	B2	20001109		
EP 931063	A1	19990728	EP 1997-937586	19970816
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1227542	A	19990901	CN 1997-197128	19970816
BR 9712808	A	19991123	BR 1997-12808	19970816
JP 2000505098	T2	20000425	JP 1998-512167	19970816
JP 3296437	B2	20020702		
NZ 334476	A	20000526	NZ 1997-334476	19970816
IL 127798	A1	20030731	IL 1997-127798	19970816
CN 1496980	A	20040519	CN 2002-2002132061	19970816
RU 2237661	C2	20041010	RU 1999-106782	19970816
ZA 9707475	A	19980219	ZA 1997-7475	19970820
CA 2215013	AA	19980306	CA 1997-2215013	19970904
CA 2215013	C	20020305		
US 6008231	A	19991228	US 1997-925326	19970908
TW 550256	B	20030901	TW 1997-86112985	19970930
NO 9901071	A	19990304	NO 1999-1071	19990304
NO 314725	B1	20030512		
US 6344467	B1	20020205	US 1999-409263	19990930
US 2002161025	A1	20021031	US 2002-58836	20020130
NO 2003000481	A	19990304	NO 2003-481	20030130
US 2003207892	A1	20031106	US 2003-402931	20030401
US 6919344	B2	20050719		
PRIORITY APPLN. INFO.:			DE 1996-19636150	A 19960906
			WO 1997-EP4474	W 19970816
			US 1997-925326	A3 19970908
			US 1999-409263	A3 19990930
			US 2002-58836	B1 20020130
OTHER SOURCE(S):	MARPAT 128:217285			
GI				



I

AB The title compds. [I; R = H, (un)substituted C1-6 alkyl; R1 = (un)substituted Ph, pyridyl, pyrimidinyl, etc.; RR1 = atoms to close (N-substituted) piperazine ring; R2 = H, (un)substituted C1-6 alkyl, (un)substituted benzoyl; R3, R4 = H, OH, C1-6 alkyl, C3-7 cycloalkyl, halo, NO2, amino, benzyloxy, etc.; Z = O, S] and their acid salts were prepared, e.g., by N-alkylation of indoles with R2-bearing reactants followed by acylation with a dicarbonyl halide and amidation of the remaining acid halide function. For example, a title compound I (R = R3 = R4 = H, R1 = 4-pyridyl, R2 = 4-FC6H4CH2, Z = O) (preparation by benzylation of indole with 4-FC6H4CH2Cl, acylation of the intermediate with (COCl)<sub>2</sub> and amidation of the acyl chloride with 4-aminopyridine given) at 10 mg/kg i.p. in guinea pigs gave 55.4% inhibition of allergen-induced late-phase eosinophilia, vs. 47.0 for cyclosporin A.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 22 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:534403 HCAPLUS

DOCUMENT NUMBER: 125:221765

TITLE: Ring-rearrangement during the Mitsunobu alkylation of phthalazinones and indazolols

AUTHOR(S): Knaack, Martina; Fleischhauer, Ilona; Charpentier, Patricia; Emig, Peter; Kutscher, Bernhard; Mueller, Arndt

CORPORATE SOURCE: Degussa A.-G., Hanau, D-63403, Germany

SOURCE: Liebigs Annalen (1996), (9), 1477-1482

CODEN: LANAEM; ISSN: 0947-3440

PUBLISHER: VCH

DOCUMENT TYPE: Journal

LANGUAGE: German

AB The Mitsunobu alkylation of substituted phthalazinones and indazolols with cyclic hydroxy- and hydroxymethyl-substituted amines was investigated. In addition to the expected derivs. ring-narrowed and ring-enlarged rearrangement products were isolated and characterized by NMR. The occurrence of these products is explained by the existence of a bicyclic intermediate. The results of the reaction of phthalazinones with optically active amine compds. show a stereospecific reaction mechanism. The reaction of the phthalazinones leads to N-substituted products, while in the case of the indazolols O-substituted derivs. were isolated. A postulated bicyclic intermediate, 1-methyl-1-azoniabicyclo[3.2.0]heptane, was synthesized as chloride.

L16 ANSWER 23 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:273624 HCAPLUS

DOCUMENT NUMBER: 124:316986

TITLE: Preparation of N-benzylindoles and -benzopyrazoles with antiasthmatic, antiallergic, antiinflammatory, and immunomodulating activity.

INVENTOR(S): Le Baut, Guillaume; Fouchard, Fabienne; Kutscher,



Bernhard; **Emig, Peter**; Schmidt, Juergen;  
 Szelenyi, Stefan; Fleischhauer, Ilona  
 PATENT ASSIGNEE(S): Asta Medica Ag, Germany  
 SOURCE: Ger. Offen., 14 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19511916	A1	19960208	DE 1995-19511916	19950331
CA 2195850	AA	19960215	CA 1995-2195850	19950720
WO 9604266	A2	19960215	WO 1995-EP2867	19950720
WO 9604266	A3	19960517		
W: AU, BR, BY, CA, CN, CZ, FI, HU, JP, KR, MX, NO, NZ, PL, RU, SI, SK, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9531626	A1	19960304	AU 1995-31626	19950720
EP 775131	A2	19970528	EP 1995-927679	19950720
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 10503501	T2	19980331	JP 1995-506137	19950720
TW 434227	B	20010516	TW 1995-84107752	19950726
ZA 9506382	A	19960313	ZA 1995-6382	19950731
IL 114795	A1	19991130	IL 1995-114795	19950801
EG 21559	A	20011231	EG 1995-644	19950801
NO 9700412	A	19970227	NO 1997-412	19970130
FI 9701334	A	19970401	FI 1997-1334	19970401
US 5965582	A	19991012	US 1997-776616	19970512
PRIORITY APPLN. INFO.:			DE 1994-4427393	A1 19940803
			DE 1995-19511916	A 19950331
			WO 1995-EP2867	W 19950720

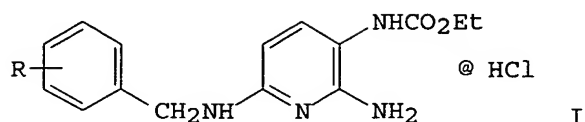
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. [I, II; R1, R10, R11, R12 = alkyl, cycloalkyl, alkoxy, (substituted) aryl, aroyl, quinolylmethyl, etc.; R2, R3 = H, alkyl, cycloalkyl, NO2, amino; R4 = H, alkyl, cycloalkyl; R5 = N-alkyl-2-pyrrolidinyl, amino; W = CH, NH; Y = O, S; X = CH, N, bond], were prepared Thus, title compound (III), prepared from indole-3-acetic acid by benzylation with 4-fluorobenzyl chloride, partial hydrolysis with NaOH in H2O/EtOH, and amidation with 4-aminopyridine/DCC, inhibited allergen-induced histamine release in rat mast cells with IC50 = 0.016  $\mu$ mol/L.

L16 ANSWER 24 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1994:605183 HCAPLUS  
 DOCUMENT NUMBER: 121:205183  
 TITLE: Synthesis and Quantitative Structure-Activity Relationships of Anticonvulsant 2,3,6-Triaminopyridines  
 AUTHOR(S): Seydel, Joachim K.; Schaper, Klaus-J.; Coats, Eugene A.; Cordes, Hans P.; **Emig, Peter**; Engel, Juergen; Kutscher, Bernhard; Polymeropoulos, Emmanuel

E.  
 CORPORATE SOURCE: Borstel Research Institute, Borstel, 23845, Germany  
 SOURCE: Journal of Medicinal Chemistry (1994), 37(19), 3016-22  
 CODEN: JMCMAR; ISSN: 0022-2623  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB The synthesis of 2,3,6-triaminopyridine derivs., , e.g. I (R = H, 3-F, 4-Cl, 4-Ac, 4-NHAc, 2-Me, 2-OH, 4-CF3, 2,4-F2, 2,4-Me2, 2,6-Me2, 2,4,6-Me3), representing a unique chemical structure for anticonvulsants, is described. The synthetic program was performed (a) to identify more potent analogs, (b) to determine structural properties controlling potency as well as neurotoxicity, and (c) to reduce the requirements for animal testing. As a result, besides other structural properties, the overall mol. lipophilicity (log k', octanol-coated column) explained changes in anticonvulsant potency and neurotoxicity. Mimicking the interaction of the amphiphilic triaminopyridines with biol. membranes, NMR expts. in the presence of lecithin vesicles were conducted in order to measure the phospholipid-binding parameter log  $\Delta(1/T_2)$ . Replacement of log k' with log  $\Delta(1/T_2)$  in the correlation anal. afforded a more significant equation describing the anticonvulsant activity of 21 derivs.

L16 ANSWER 25 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:569743 HCAPLUS  
 DOCUMENT NUMBER: 121:169743  
 TITLE: QSAR analysis of time- and dose-dependent in vivo drug effects using artificial neural networks  
 AUTHOR(S): Schapper, Klaus-Juergen; Wiese, Michael; Dieter, Reinhold; ~~Emig~~, Peter; Engel, Juergen; Kutscher, Bernhard; Polymeropoulos, Emmanuel E.  
 CORPORATE SOURCE: Borstel Res. Inst., Borstel, D-2061, Germany  
 SOURCE: Trends QSAR Mol. Modell. 92, Proc. Eur. Symp. Struct.-Act. Relat.: QSAR Mol. Modell., 9th (1993), Meeting Date 1992, 546-9. Editor(s): Wermuth, Camille-Georges. ESCOM: Leiden, Neth. CODEN: 59XTAS  
 DOCUMENT TYPE: Conference  
 LANGUAGE: English  
 AB QSAR anal. of time- and dose-dependent in vivo anticonvulsant activities of triaminobenzenes was carried out. Property-dependent activities were estimated Complete dos-response curves were obtained.

L16 ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:426878 HCAPLUS  
 DOCUMENT NUMBER: 121:26878  
 TITLE: Pharmaceutical composition consisting of flupirtine and morphine for the treatment of pain and to avoid a morphine addiction  
 INVENTOR(S): Nickel, Bernd; Lobisch, Michael; Szelenyi, Stefan; Engel, Juergen; ~~Emig~~, Peter; Pergande, Gabriela

PATENT ASSIGNEE(S): ASTA Medica AG, Germany  
 SOURCE: Eur. Pat. Appl., 10 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 595311	A1	19940504	EP 1993-117472	19931028
EP 595311	B1	19970122		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
DE 4236752	A1	19940505	DE 1992-4236752	19921030
US 5521178	A	19960528	US 1993-141678	19931027
AT 147979	E	19970215	AT 1993-117472	19931028
ES 2099344	T3	19970516	ES 1993-117472	19931028
CA 2102072	AA	19940501	CA 1993-2102072	19931029
CA 2102072	C	20050104		
BR 9304431	A	19940607	BR 1993-4431	19931029
JP 06211663	A2	19940802	JP 1993-271730	19931029
JP 3665354	B2	20050629		
HU 66085	A2	19940928	HU 1993-3089	19931029
HU 219907	B	20010928		

PRIORITY APPLN. INFO.: DE 1992-4236752 A 19921030  
 AB Coadministration of flupirtine and morphine results in additive analgesic activity, reduced dependence on morphine, and no development of tolerance to flupirtine. Thus, the excitation, rearing behavior, and rigidity seen in rats after withdrawal from morphine in long-term expts. were markedly less in rats which had been injected with morphine and flupirtine. A preferred dosage form was a tablet containing 50-500 mg flupirtine and 10-250 mg morphine as salts.

L16 ANSWER 27 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:560063 HCAPLUS

DOCUMENT NUMBER: 119:160063

TITLE: New triaminopyridines with a central analgesic activity

AUTHOR(S): Emig, P.; Nickel, B.; Weischer, C.-H.; Szelenyi, I.; Engel, J.

CORPORATE SOURCE: Forschung Asta Med. AG, Frankfurt/Main, Germany

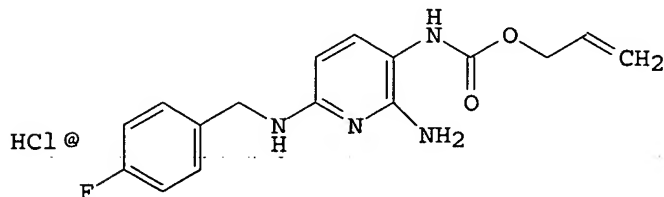
SOURCE: Arzneimittel-Forschung (1993), 43(6), 627-31

CODEN: ARZNAD; ISSN: 0004-4172

DOCUMENT TYPE: Journal

LANGUAGE: German

GI



I

AB 2-Amino-3-[[[(3-propenyl)oxy]carbonyl]amino]-6-[(4-fluorobenzyl)amino]pyridine hydrochloride [D-19050; 2-propenyl [2-amino-6-[[[(4-fluorophenyl)methyl]amino]-3-pyridinyl]carbamate] (I) is a centrally and peripherally acting analgesic with rapid onset, long duration of action and a good therapeutic range. D-19050 can be obtained in a 5-step-preparation starting from 2,6-dichloropyridine. I is a flupirtine analog.

L16 ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:120908 HCAPLUS  
 DOCUMENT NUMBER: 116:120908  
 TITLE: Flupirtine as spasmolytic  
 INVENTOR(S): Lobisch, Michael; Venhaus, Ralph; Nickel, Bernd; Szelenyi, Istvan; Engel, Juergen; **Emig, Peter**  
 PATENT ASSIGNEE(S): Asta Pharma A.-G., Germany  
 SOURCE: Ger. Offen., 7 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4122166	A1	19920116	DE 1991-4122166	19910704
IN 172468	A	19930814	IN 1991-CA421	19910604
EP 467164	A2	19920122	EP 1991-111124	19910704
EP 467164	A3	19920415		
EP 467164	B1	19960131		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
EP 659410	A2	19950628	EP 1995-101189	19910704
EP 659410	A3	19951025		
EP 659410	B1	20011017		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AT 133564	E	19960215	AT 1991-111124	19910704
ES 2082887	T3	19960401	ES 1991-111124	19910704
AT 206919	E	20011115	AT 1995-101189	19910704
ES 2164111	T3	20020216	ES 1995-101189	19910704
CZ 280879	B6	19960417	CZ 1991-2101	19910708
SK 279567	B6	19990111	SK 1991-2101	19910708
RO 108220	B1	19940331	RO 1991-147972	19910709
US 5162346	A	19921110	US 1991-726408	19910710
CA 2046943	AA	19920115	CA 1991-2046943	19910712
CA 2046943	C	19960312		
NO 9102758	A	19920115	NO 1991-2758	19910712
AU 9180403	A1	19920116	AU 1991-80403	19910712
AU 634073	B2	19930211		
ZA 9105466	A	19920429	ZA 1991-5466	19910712
HU 59313	A2	19920528	HU 1991-2359	19910712
HU 206973	B	19930301		
IL 98810	A1	19960119	IL 1991-98810	19910712
RU 2070408	C1	19961220	RU 1991-5001150	19910712
CN 1058716	A	19920219	CN 1991-104030	19910713
CN 1070700	B	20010912		
KR 182811	B1	19990501	KR 1991-11967	19910713
JP 05032627	A2	19930209	JP 1991-188472	19910729
US 5284861	A	19940208	US 1992-890730	19920601
LV 10048	B	19950620	LV 1992-173	19921027
LT 3593	B	19951227	LT 1993-919	19930903
PRIORITY APPLN. INFO.:			DE 1990-4022442	A1 19900714

EP 1991-111124 A3 19910704  
US 1991-726408 A3 19910710

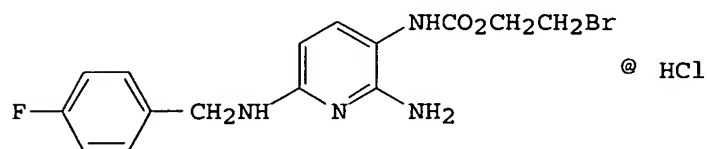
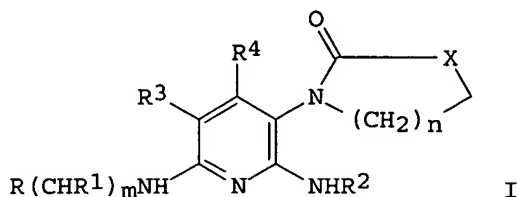
AB Flupirtine (I) is a spasmolytic for muscles. I may be used for increasing the tonus of skeletal muscles in parkinsonism, optionally in combination with known drugs for the treatment of parkinsonism, such as (-)-deprenyl, biperiden or L-DOPA. I.p. administration of 5 mg I + 5 mg L-DOPA/kg decreased in vivo the reserpine-induced rigidity of the rat flexor muscle.

L16 ANSWER 29 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:235286 HCAPLUS  
DOCUMENT NUMBER: 112:235286  
TITLE: Preparation of (aminopyridyl)oxazolidinones and their analogs as antiepileptics  
INVENTOR(S): Engel, Juergen; Emig, Peter; Nickel, Bernd; Szelenyi, Istvan  
PATENT ASSIGNEE(S): Asta Pharma A.-G., Fed. Rep. Ger.  
SOURCE: Ger. Offen., 8 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3915184	A1	19891130	DE 1989-3915184	19890510
EP 343429	A1	19891129	EP 1989-108369	19890510
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
DK 8902326	A	19891117	DK 1989-2326	19890512
AU 8934819	A1	19891116	AU 1989-34819	19890515
JP 02017186	A2	19900122	JP 1989-120578	19890516
US 4923858	A	19900508	US 1989-352287	19890516
PRIORITY APPLN. INFO.:			DE 1988-3816629	A1 19880516
OTHER SOURCE(S):			CASREACT 112:235286; MARPAT 112:235286	

GI



AB The title compds. [I; R = (substituted) aryl; R1, R2 = H, alkyl; R3, R4 = H, alkyl, OH, alkoxy, etc.; X = O, S, (substituted) imino; m, n = 1, 2, 3] are prepared. Bromoethyl pyridylcarbamate II in EtOH was treated with NH3 in EtOH at room temperature for 24 h to give I [R = p-FC6H4, R1-R4 = H, X = O, m = n = 1]. In an example using the maximum elec. shock test, the ED50 for I (no specific compound mentioned) was 56 mg/kg in mice. Capsules and

suppositories containing I were formulated.

L16 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:453587 HCAPLUS  
DOCUMENT NUMBER: 111:53587  
TITLE: Determination of total bilirubin in serum and test strip determination for bilirubinemia, urobilinogenuria, and proteinuria: interference from the analgesic flupirtin  
AUTHOR(S): Thomas, L.; Riethmueller-Winzen, H.; Niebch, G.; Emig, P.; Harleman, J. H.  
CORPORATE SOURCE: Zentrallab., Krankenhaus Nordwest, Frankfurt/Main, D-6900/90, Fed. Rep. Ger.  
SOURCE: Laboratoriumsmedizin (1989), 13(4), 136-41  
CODEN: LABOD3; ISSN: 0342-3026  
DOCUMENT TYPE: Journal  
LANGUAGE: German

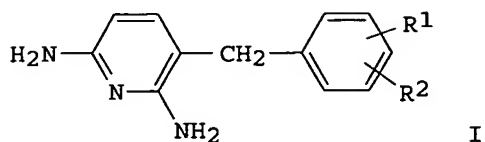
AB Test strips (Ames-N-multistix, Combur-9-Test, Rapignost-Total-Screen) gave false-pos. results for bilirubin (I), urobilinogen (II), and protein (III) detns. in human urine in the presence of flupirtine (IV), either following in vitro spiking of samples or after daily oral administration of the drug to patients. For I and II detns., strongly colored azo-type reactions with the indicator reagents were observed; for III detns. the reason for this interference was not found, although expts. indicated that the biuret determination of III was not influenced by IV. Test-strip detns. of total blood serum I were also influenced by IV (i.e. they indicated increased I values in a IV dose-dependent manner) which depended upon assay system used, but at the maximum serum levels of IV expected, this interference was clin. insignificant.

L16 ANSWER 31 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:492815 HCAPLUS  
DOCUMENT NUMBER: 109:92815  
TITLE: Preparation of 2,6-diamino-3-(halobenzyl)pyridines as analgesics and antipyretics  
INVENTOR(S): Emig, Peter; Engel, Juergen; Scheffler, Gerhard; Weischer, Carl Heinrich; Nickel, Bernd  
PATENT ASSIGNEE(S): Asta Pharma A.-G., Fed. Rep. Ger.  
SOURCE: Ger. Offen., 5 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DE 3637829	A1	19880511	DE 1986-3637829	19861106
CN 87106966	A	19880831	CN 1987-106966	19871019
EP 266711	A1	19880511	EP 1987-116036	19871031
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
FI 8704875	A	19880507	FI 1987-4875	19871104
DD 270903	A5	19890816	DD 1987-308667	19871104
DD 276280	A5	19900221	DD 1987-323143	19871104
PL 149462	B1	19900228	PL 1987-268592	19871104
DK 8705814	A	19880507	DK 1987-5814	19871105
NO 8704617	A	19880509	NO 1987-4617	19871105
AU 8780826	A1	19880512	AU 1987-80826	19871105
AU 596708	B2	19900510		

JP 63132875      A2      19880604      JP 1987-278411      19871105  
 ZA 8708324      A      19880629      ZA 1987-8324      19871105  
 HU 45502      A2      19880728      HU 1987-4965      19871105  
 HU 197882      B      19890628  
 US 4851420      A      19890725      US 1987-116807      19871105  
 PRIORITY APPLN. INFO.:      DE 1986-3637829      A      19861106  
 OTHER SOURCE(S):      CASREACT 109:92815; MARPAT 109:92815  
 GI



AB The title compds. (I; R1 = F; R2 = H, Cl) were prepared as analgesics and antipyretics (no data). 2,6-Diaminopyridine was slowly heated to melting and 4-FC6H4CH2Cl was added dropwise followed by heating at 130-150° for 4 h to give 59% 2,6-diamino-3-(4-fluorobenzyl)pyridine.

L16 ANSWER 32 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1987:50057 HCAPLUS  
 DOCUMENT NUMBER: 106:50057  
 TITLE: 2-Amino-3-nitro-6-(4-fluorobenzylamino)pyridine and  
 2-amino-3-carbethoxyamino-6-(4-fluorobenzylamino)pyridine  
 INVENTOR(S): Orth, Winfried; Engel, Juergen; **Emig, Peter**;  
 Scheffler, Gerhard; Pohle, Hans  
 PATENT ASSIGNEE(S): Degussa A.-G., Fed. Rep. Ger.  
 SOURCE: Ger. Offen., 11 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3608762	A1	19861002	DE 1986-3608762	19860315
NO 8600825	A	19860924	NO 1986-825	19860305
EP 199951	A2	19861210	EP 1986-103517	19860315
EP 199951	A3	19871014		
EP 199951	B1	19910123		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
AT 60322	E	19910215	AT 1986-103517	19860315
DK 8601268	A	19860924	DK 1986-1268	19860319
DK 162215	B	19910930		
DK 162215	C	19920316		
FI 8601183	A	19860924	FI 1986-1183	19860320
FI 84819	B	19911015		
FI 84819	C	19920127		
AU 8654997	A1	19860925	AU 1986-54997	19860321
AU 579922	B2	19881215		
ZA 8602138	A	19861126	ZA 1986-2138	19860321
BR 8601283	A	19861202	BR 1986-1283	19860321
ES 553222	A1	19870116	ES 1986-553222	19860321
DD 246761	A5	19870617	DD 1986-288169	19860321

CS 259887	B2	19881115	CS 1986-1986	19860321
PL 146631	B1	19890228	PL 1986-258543	19860321
IL 78218	A1	19891215	IL 1986-78218	19860321
CA 1273343	A1	19900828	CA 1986-504732	19860321
JP 61221172	A2	19861001	JP 1986-64292	19860324
JP 01046510	B4	19891009		
HU 40418	A2	19861228	HU 1986-1216	19860324
HU 206679	B	19921228		
US 4785110	A	19881115	US 1986-843253	19860324
PRIORITY APPLN. INFO.:			DE 1985-3510623	A1 19850323
			EP 1986-103517	A 19860315

OTHER SOURCE(S): CASREACT 106:50057

AB The title compds. (I and II resp.) were prepared Thus, 25-amino-3-nitro-6-methoxy-pyridine was condensed with 4-FC6H4CH2NH2 to give 95.2% I. I (26.2 g) was reduced with Raney-Ni in dioxane and acylated with ClCO2Et to give 19 g II.

L16 ANSWER 33 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1986:632448 HCAPLUS

DOCUMENT NUMBER: 105:232448

TITLE: Preparation of flupirtine gluconate salt for injection

INVENTOR(S): Hettche, Helmut; ~~Emig~~, Peter; Engel, Juergen

PATENT ASSIGNEE(S): Degussa A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen., 15 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

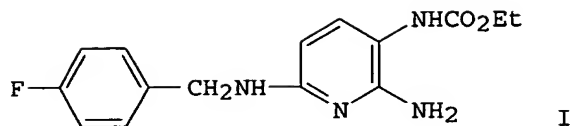
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3416609	A1	19851107	DE 1984-3416609	19840505
EP 160865	A2	19851113	EP 1985-104746	19850419
EP 160865	A3	19860312		
EP 160865	B1	19880420		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
AT 33638	E	19880515	AT 1985-104746	19850419
SU 1398772	A3	19880523	SU 1985-3884101	19850426
CS 248743	B2	19870212	CS 1985-3157	19850430
US 4673666	A	19870616	US 1985-729413	19850501
DK 8501987	A	19851106	DK 1985-1987	19850502
DK 157016	B	19891030		
DK 157016	C	19900326		
DD 236927	A5	19860625	DD 1985-275890	19850502
FI 8501752	A	19851106	FI 1985-1752	19850503
FI 80443	B	19900228		
FI 80443	C	19900611		
NO 8501772	A	19851106	NO 1985-1772	19850503
AU 8541943	A1	19851107	AU 1985-41943	19850503
ES 542817	A1	19851216	ES 1985-542817	19850503
ZA 8503351	A	19851224	ZA 1985-3351	19850503
HU 37758	A2	19860228	HU 1985-1691	19850503
HU 193753	B	19871130		
IL 75086	A1	19880331	IL 1985-75086	19850503
CA 1263398	A1	19891128	CA 1985-480723	19850503
JP 60239469	A2	19851128	JP 1985-95714	19850507
JP 01044185	B4	19890926		

PRIORITY APPLN. INFO.:

DE 1984-3416609	A	19840505
EP 1985-104746	A	19850419



GI



I

AB Flupirtine (I) gluconate salt is prepared by reacting I with gluconic acid or gluconic acid- $\delta$ -lactone to improve its solubility and stability. A parenteral solution can be formulated using solvents such as polyethylene glycol, glycofurol, and water. Thus I was added to a solution of gluconic acid obtained by hydrolysis of gluconic acid- $\delta$ -lactone. A mixture containing I gluconate salt, PEG, and NaHSO<sub>3</sub> was microfiltered and stored in colorless ampules.

L16 ANSWER 34 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:610967 HCAPLUS

DOCUMENT NUMBER: 101:210967

TITLE: Ethylenediamine and guanidine derivatives

INVENTOR(S): Emig, Peter; Scheffler, Gerhard; Thiemer, Klaus; Weischer, Carl Heinrich

PATENT ASSIGNEE(S): Degussa A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen., 64 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

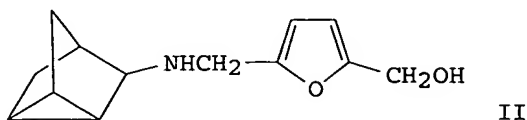
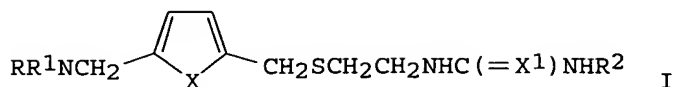
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

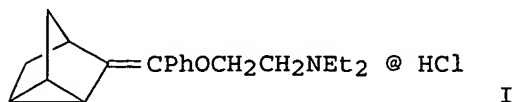
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3343884	A1	19840614	DE 1983-3343884	19831205
DE 3343884	C2	19910711		
NL 8303965	A	19840702	NL 1983-3965	19831117
SU 1222196	A3	19860330	SU 1983-3663583	19831121
FR 2537582	A1	19840615	FR 1983-19390	19831205
FR 2537582	B1	19861205		
BE 898403	A1	19840606	BE 1983-47911	19831206
AU 8322138	A1	19840614	AU 1983-22138	19831206
AU 564254	B2	19870806		
GB 2132615	A1	19840711	GB 1983-32433	19831206
GB 2132615	B2	19860702		
DD 216013	A5	19841128	DD 1983-257557	19831206
DK 8305633	A	19840609	DK 1983-5633	19831207
DK 163732	B	19920330		
DK 163732	C	19920831		
FI 8304481	A	19840609	FI 1983-4481	19831207
SE 8306764	A	19840609	SE 1983-6764	19831207
ZA 8309107	A	19840725	ZA 1983-9107	19831207
ES 527864	A1	19840801	ES 1983-527864	19831207
HU 35255	O	19850628	HU 1983-4192	19831207
IL 70401	A1	19871030	IL 1983-70401	19831207
US 4738983	A	19880419	US 1983-558984	19831207
CA 1257867	A1	19890725	CA 1983-442695	19831207
AT 8304278	A	19900115	AT 1983-4278	19831207
AT 390952	B	19900725		

JP 59112980	A2	19840629	JP 1983-230710	19831208
JP 05072386	B4	19931012		
CS 241141	B2	19860313	CS 1983-9224	19831208
CH 657850	A	19860930	CH 1983-6576	19831208
PRIORITY APPLN. INFO.:			DE 1982-3245387	A1 19821208
OTHER SOURCE(S):	MARPAT 101:210967			
GI				



AB The title compds. [I; R = polycycloalkyl, (un)substituted alkyl, cycloalkyl; R1 = H, (un)substituted alkyl; R2 = H, alkenyl, alkynyl, cycloalkyl, 2-[[[5-[(dimethylamino)methyl]-2-furanyl]methyl]thio]ethyl, (un)substituted alkyl; X = O, S; X1 = R3CH, RN; R3 = NO2, cyano] were prepared. Thus, 2-furanmethanol was aminomethylated with R4NH2 (R4 = tricyclo[2.2.1.2.2]hept-3-yl] and paraformaldehyde to give II, which was condensed with HSCH2CH2NH.HCl, O2NC:C(SMe)2 and MeNH2 to give I (R = R4, R1 = H, R2 = Me, X = O, X1 = O2NCH). I are as effective as ranitidine in inhibiting stomach secretion in rats.

L16 ANSWER 35 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1983:143000 HCAPLUS  
 DOCUMENT NUMBER: 98:143000  
 TITLE: Synthesis and structure of new basic enol ethers  
 AUTHOR(S): Risch, N.; Emig, P.; Scheffler, G.; Pohle, H.; Henkel, G.  
 CORPORATE SOURCE: Forsch. Geschaeftsber. Pharma, Degussa A.-G., Frankfurt/Main, Fed. Rep. Ger.  
 SOURCE: Arzneimittel-Forschung (1982), 32(11), 1409-11  
 CODEN: ARZNAD; ISSN: 0004-4172  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 OTHER SOURCE(S): CASREACT 98:143000  
 GI



AB Enol ethers (E)- and (Z)-I are spasmolytics and also have antiallergy and antidepressant properties. Treating bicyclo[2.2.1]hepta-2,5-diene in CH<sub>2</sub>Cl<sub>2</sub> with HCl(g) 6 h gave 88.2% a mixture of II and III (R = Cl). Grignard reaction of the mixture gave III [R = PhC(:NH)], hydrolysis of which gave 93.8% III (R = Bz). This, with NaNH<sub>2</sub> and Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>Cl in refluxing PhMe gave 81.7% free base, which was converted to I. X-ray anal. of (E)-I confirmed the structure.

L16 ANSWER 36 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1976:89707 HCAPLUS

DOCUMENT NUMBER: 84:89707

TITLE: Basic enol ethers and their salts

INVENTOR(S): Emig, Peter; Pohle, Hans; Scheffler, Gerhard; Brock, Norbert; Lenke, Hans D.; Pohl, Joerg

PATENT ASSIGNEE(S): Asta-Werke A.-G. Chemische Fabrik, Fed. Rep. Ger.

SOURCE: Ger. Offen., 35 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2413814	A1	19751002	DE 1974-2413814	19740322
DE 2413814	C3	19791004		
DE 2413814	B2	19790201		
CH 610291	A	19790412	CH 1975-2745	19750305
SE 7502607	A	19750923	SE 1975-2607	19750307
SE 421916	B	19820208		
SE 421916	C	19820527		
ZA 7501415	A	19760526	ZA 1975-1415	19750307
IL 46786	A1	19771130	IL 1975-46786	19750310
US 4065501	A	19771227	US 1975-557535	19750312
AU 7579012	A1	19760916	AU 1975-79012	19750313
GB 1446164	A	19760818	GB 1975-10992	19750317
DD 119208	C	19760412	DD 1975-184851	19750318
AT 7502073	A	19770315	AT 1975-2073	19750318
AT 339878	B	19771110		
CS 185682	P	19781031	CS 1975-1816	19750318
CS 185698	P	19781031	CS 1977-914	19750318
CA 1054152	A1	19790508	CA 1975-222446	19750318
DK 7501111	A	19750923	DK 1975-1111	19750319
DK 141818	B	19800623		
DK 141818	C	19801110		
JP 50129539	A2	19751013	JP 1975-33471	19750319
JP 58029777	B4	19830624		
FR 2264523	A1	19751017	FR 1975-8742	19750320
FR 2264523	B1	19790629		
ES 435796	A1	19761216	ES 1975-435796	19750320
PL 97364	P	19780228	PL 1975-178944	19750320
PL 97365	P	19780228	PL 1975-195370	19750320
BE 826950	A1	19750716	BE 1975-2054220	19750321
FI 7500856	A	19750923	FI 1975-856	19750321
FI 62662	B	19821029		
FI 62662	C	19830210		
NL 7503414	A	19750924	NL 1975-3414	19750321
SU 614743	D	19780705	SU 1975-2115295	19750321
HU 173792	P	19790828	HU 1975-AA807	19750321

AT 7606966	A	19770215	AT 1976-6966	19760920
AT 339278	B	19771010		
SU 639444	D	19781225	SU 1977-2440657	19770124
US 4124716	A	19781107	US 1977-842092	19771014
PRIORITY APPLN. INFO.:			DE 1974-2413814	A 19740322
			US 1975-557535	A2 19750312
			AT 1975-2073	A 19750318

OTHER SOURCE(S): MARPAT 84:89707

GI For diagram(s), see printed CA Issue.

AB The enol ethers I (R = Ph, substituted phenyl, thienyl, pyridyl; R1 = H, Me, Et; R2 = Me, Et; NR1R2 = pyrrolidino, morpholino; n = 2,3), useful as spasmolytics were prepared. Thus, II and Me2NCH2CH2Cl were added to a suspension of NaNH2 in boiling PhMe, and the mixture was refluxed for 1.5 hr to give 76% I (R = Ph, R1 = R2 = Me, n = 2). About 15 I were prepared and tested for spasmolytic activity on guinea pigs.

L16 ANSWER 37 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1970:477580 HCAPLUS

DOCUMENT NUMBER: 73:77580

TITLE: Nucleosides. X. Synthesis of dipeptidyl aminosugar nucleosides structurally related to gougerotin

AUTHOR(S): Lichtenthaler, Frieder W.; Trummlitz, G.; **Emig, Peter**

CORPORATE SOURCE: Inst. Org. Chem., Tech. Hochsch., Darmstadt, Fed. Rep. Ger.

SOURCE: Tetrahedron Letters (1970), (24), 2061-4  
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB N-tert-Butoxycarbonylsarcosine, prepared from sarcosine and 2,4,5-Cl3C6H2O2COBu-tert, was treated with D-serine Me ester-HCl to give N-tert-butoxycarbonylsarcosyl-D-serine Me ester which was converted into the corresponding hydrazide. The latter treated with BuNO2 in DMF gave the corresponding azide which was coupled with 1-(3-amino-3-deoxy-β-D-glucopyranosyl)cytosine (Luebke, K., et al., 1964) to give a tert-butoxycarbonyl-blocked dipeptidyl nucleoside which on removal of the protecting group with F3CCO2H gave 1-[3-(sarcosyl-D-serylamido)-3-deoxy-β-D-glucopyranosyl]cytosine (I). Similarly prepared was II.

L16 ANSWER 38 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1969:106817 HCAPLUS

DOCUMENT NUMBER: 70:106817

TITLE: Nucleosides. VIII. Configuration assignment of sugars and hexopyranosyl nucleosides by the acetyl-resonance rule

AUTHOR(S): Lichtenthaler, Frieder W.; Bambach, Gerd; **Emig, Peter**

CORPORATE SOURCE: Tech. Hochsch. Darmstadt, Darmstadt, Fed. Rep. Ger.

SOURCE: Chemische Berichte (1969), 102(3), 994-1004

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

AB The 1H N.M.R. spectra were recorded for per-O-acetyl-D-aldopyranoses and the corresponding per-O-acetyl-2-amino-2-deoxy-D-aldopyranoses with per-O-D-gluc, D-galacto, and D-manno configurations in CDCl3 and (D3C)2SO. Results are tabulated and solvent shifts were determined. Solvent shifts of the Ac protons were small (≤0.05 ppm.) in comparison with diamagnetic solvent shifts, .apprx.0.15 ppm., of the NHAc group. In fully acetylated hexopyranosyl nucleosides, the anisotropy of the base causes a

acetamido groups.

L16 ANSWER 41 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1967:454388 HCAPLUS

DOCUMENT NUMBER: 67:54388

TITLE: N.M.R. studies on sugars and cyclanols. III.  
Configuration of C-methyl-branched sugars and  
cyclanols at the branching point

AUTHOR(S): Lichtenthaler, Frieder W.; Emig, P.

CORPORATE SOURCE: Tech. Hochsch., Darmstadt, Fed. Rep. Ger.

SOURCE: Tetrahedron Letters (1967), (7), 577-82

CODEN: TELEAY; ISSN: 0040-4039

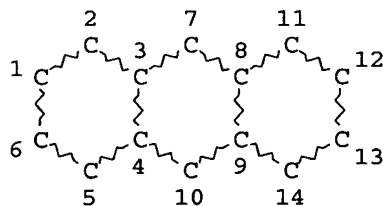
DOCUMENT TYPE: Journal

LANGUAGE: English

AB cf. CA 64: 19740c. Summary of N.M.R. studies of peracetates of sugars, cyclanols, amino sugars, and amino-cyclanols in CDCl<sub>3</sub> showed that the signal positions of acetoxy and acetamido resonances offer a convenient and generally surprisingly accurate means for configurational and conformational assignments. In view of this relationship similar relations would be expected for CMeOAc and CMeNHAc groups. In a summary of the chemical shifts in CDCl<sub>3</sub> of  $\delta$  C-Me branched cyclanol acetates the differences in chemical shift between the equatorial and axial C-Me protons was small. However, the Me protons of the AcO group at the branching point showed differences of about 0.1 ppm. between axial and equatorial orientation showing the replacement of a ring H atom by a Me group causes an upward shift of the AcO signal. Accordingly, the configuration at the branching point can be deduced from the signal position of the AcO group attached to the C-Me branch of a cyclanol. A similar upward shift can be assumed for the Me protons of acetamido groups when an Me group is substituted for the ring H atom. The expected range for axial C-Me acetamido groups would thus be 8.07-8.14  $\tau$  as compared with 8.13-8.22  $\tau$  for their equatorial counterparts. Of the 7 C-Me branched aminocyclanol and amino sugar acetates which have been prepared and whose configuration at the branching point had not been assigned, the acetamido signals appear within the very small range of 0.05 ppm. and on the basis of their chemical shifts (8.15-8.20  $\tau$ ) indicated an equatorial acetamido group in each compound and permitted the configurational assignments given. Since all compds. were prepared by cyclization of a dialdehyde with EtNO<sub>2</sub>, it was concluded that the EtNO<sub>2</sub> cyclization proceeds analogous to the MeNO<sub>2</sub>-dialdehyde cyclization, with the NO<sub>2</sub> group preferentially, if not exclusively, attaining the equatorial position in the cyclization step.

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L5 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

general diamagnetic shift of the vicinal 2'-acetyl signals: 0.1 ppm. for pyrimidine; 0.3 ppm. for purine. Configurations of the hexopyranosyl nucleosides were thus unambiguously determined

L16 ANSWER 39 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1969:106813 HCAPLUS

DOCUMENT NUMBER: 70:106813

TITLE: Nucleosides. VI. Nucleoside conversion in the 3'-aminohexosyl-hypoxanthine series

AUTHOR(S): Lichtenthaler, Frieder W.; Emig, Peter; Bommer, Dieter

CORPORATE SOURCE: Tech. Hochsch. Darmstadt, Darmstadt, Fed. Rep. Ger.

SOURCE: Chemische Berichte (1969), 102(3), 971-85

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

AB Cyclization of 2-O-[(R)-formyl(hypoxanthin-9-yl)methyl]-D-glyceraldehyde with MeNO<sub>2</sub> yielded 9-(3-deoxy-3-nitro-β-D-glucopyranosyl)hypoxanthine and 9-(3-deoxy-3-nitro-β-D-galactopyranosyl)hypoxanthine. The latter gave upon hydrogenation 9-(3-amino-3-deoxy-β-D-galactopyranosyl)hypoxanthine. 9-(3-Acetamido-4,6-O-benzylidene-3-deoxy-β-D-glucopyranosyl)hypoxanthine was converted into its 2-O-(methylsulfonyl) derivative which heated with NaOAc gave 9-(3-acetamido-4,6-O-benzylidene-3-deoxy-β-D-mannopyranosyl)hypoxanthine. The latter was acetylated, after the removal of the 4,6-O-benzylidene group, to give 9-(3-acetamido-2,4,6-tri-O-acetyl-3-deoxy-β-D-mannopyranosyl)hypoxanthine. Similarly was prepared 9-(3-acetamido-2,4,6-tri-O-acetyl-3-deoxy-β-D-galactopyranosyl)hypoxanthine, starting from 9-(3-acetamido)-4,6-O-benzylidene-3-deoxy-β-D-galactopyranosyl)hypoxanthine. Treatment of 9-(3-acetamido-2,4,6-tri-O-acetyl-3-deoxy-β-D-glucopyranosyl)hypoxanthine with P<sub>4</sub>S<sub>10</sub> in pyridine gave 9-(2,4,6-tri-O-acetyl-3-deoxy-3-thioacetamido-β-D-glucopyranosyl)hypoxanthine and 6-mercapto-9-(2,3,6-tri-O-acetyl-3-deoxy-3-thioacetamido-β-D-glucopyranosyl)purine (I). I was converted into the corresponding 6-(methylthio) derivative which upon ammonolysis, followed by acetylation, gave 9-(3-acetamido-2,4,6-tri-O-acetyl-3-deoxy-β-D-glucopyranosyl)adenine. The chlorination of I, followed by the addition of Me<sub>2</sub>NH gave 9-(3-acetamido-3-deoxy-β-D-glucopyranosyl)-6-(dimethylamino)purine.

L16 ANSWER 40 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1968:444143 HCAPLUS

DOCUMENT NUMBER: 69:44143

TITLE: Nuclear magnetic resonance studies on sugars and cyclanols. V. Relation between the steric orientation of O- and N-acetyl groups and the methyl resonance signal location in cyclitol and aminocyclitol polyacetates

AUTHOR(S): Lichtenthaler, F. W.; Emig, P.

CORPORATE SOURCE: Tech. Hochsch. Darmstadt, Darmstadt, Fed. Rep. Ger.

SOURCE: Carbohydrate Research (1968), 7(2), 121-37

CODEN: CRBRAT; ISSN: 0008-6215

DOCUMENT TYPE: Journal

LANGUAGE: German

AB Absorption ranges are deduced for axial and equatorial O- and N-acetyl-resonances of cyclitol and aminocyclitol peracetates on the basis of 41 (CDCl<sub>3</sub>) and 22 (Me<sub>2</sub>SO-d<sub>6</sub>) compds., allowing configurational and conformational assignments. Scope and limitations are discussed; especially application to compds. having substituents other than acetoxy and

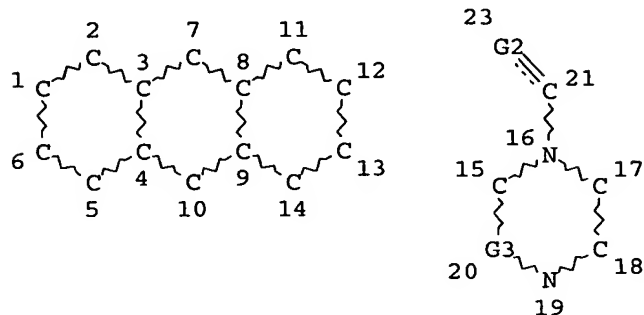
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NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L7 118852 SEA FILE=REGISTRY SSS FUL L5

L8 STR



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REP G3=(1-4) C

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

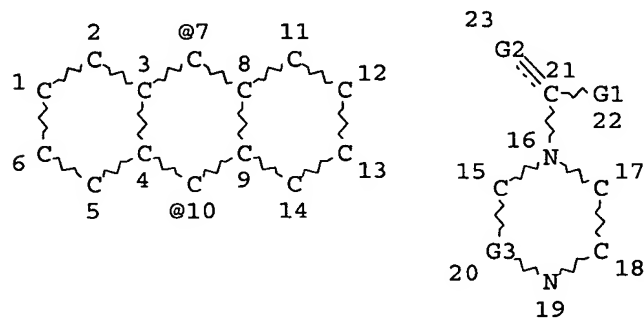
RSPEC 16

NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L9 157 SEA FILE=REGISTRY SUB=L7 SSS FUL L8

L10 STR



VAR G1=7/10

VAR G2=O/S

REP G3=(1-4) C

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 15

NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

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L12 7 SEA FILE=HCAPLUS ABB=ON PLU=ON L11

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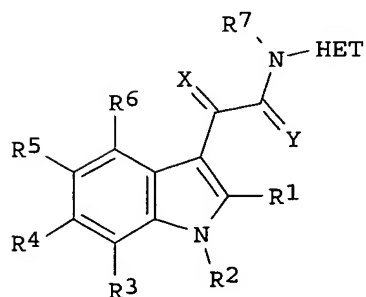
PETER"/AU)

L16 41 SEA FILE=HCAPLUS ABB=ON PLU=ON L15 NOT L12  
 L17 67 SEA FILE=HCAPLUS ABB=ON PLU=ON ("GUNTHER E"/AU OR "GUNTHER  
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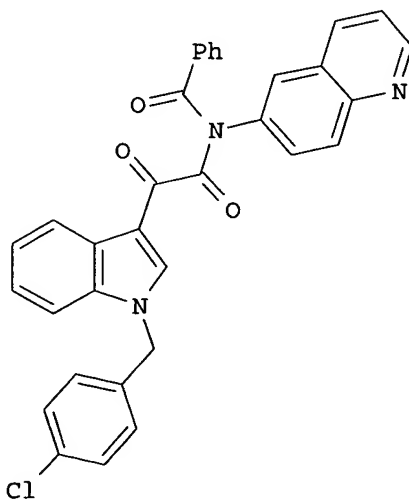
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L17 ANSWER 1 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:78242 HCAPLUS  
 DOCUMENT NUMBER: 142:176683  
 TITLE: Preparation of N-substituted indolyl-3-glyoxylamides  
 as antitumor agents  
 INVENTOR(S): Gerlach, Matthias; Schuster, Tilmann; Schmidt, Peter;  
 Baasner, Silke; Gunther, Eckhard  
 PATENT ASSIGNEE(S): Germany  
 SOURCE: U.S. Pat. Appl. Publ., 9 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005020636	A1	20050127	US 2004-892040	20040715
PRIORITY APPLN. INFO.:			US 2003-490004P	P 20030725
OTHER SOURCE(S):	MARPAT 142:176683			
GI				



I



II

AB The title compds. I [R1, R3-R6 = H, (un)substituted (cyclo)alkyl, (hetero)aryl, alkylaryl, etc.; R2 = (un)substituted alkyl, alkylaryl, alkylheteroaryl; R7 = SO2X1 (wherein X1 = dialkylamino, OH, (un)substituted (cyclo)alkyl, (hetero)aryl, etc.), COX2 (X2 = (un)substituted (hetero)aryl, alkylaryl, alkylheteroaryl), etc.; X = O, S or geminally linked H and OH; Y = O, S; HET = (un)saturated or aromatic



heterocycle comprising N, O and S which can be bonded to the amide nitrogen directly or via alkyl bridge], useful as medicaments, in particular for the treatment of tumors, were prepared General procedure for synthesis of compds. I such as II which comprises reacting 2-[1-(4-chlorobenzyl)-1H-indol-3-yl]-2-oxo-N-quinolin-6-ylacetamide with acyl chloride, was described. The compound II was tested for inhibition of selected tumor cell lines and antiproliferative action on MDR tumor cell lines (data given). The pharmaceutical composition comprising the compound I is disclosed.

L17 ANSWER 2 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:252340 HCAPLUS

DOCUMENT NUMBER: 140:264487

TITLE: Medicaments containing disorazoles and derivatives thereof for the treatment of benign and malignant tumors

INVENTOR(S): Irschik, Herbert; Jansen, Rolf; Sasse, Florenz; Baasner, Silke; Schmidt, Peter; Gunther, Eckhard

PATENT ASSIGNEE(S): Zentaris GmbH, Germany

SOURCE: PCT Int. Appl., 30 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004024149	A1	20040325	WO 2003-EP9329	20030822
W: AT, AU, BR, BY, CA, CN, CO, GE, HR, ID, IL, IN, IS, JP, KR, KZ, LT, LV, MK, MX, NO, NZ, PH, PL, RU, SG, UA, UZ, YU, ZA				
RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
CA 2438001	AA	20040224	CA 2003-2438001	20030822
AU 2003296872	A1	20040430	AU 2003-296872	20030822
US 2004106662	A1	20040603	US 2003-646904	20030822
EP 1536789	A1	20050608	EP 2003-794920	20030822
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, TR, BG, CZ, EE, HU, SK				
BR 2003013789	A	20050705	BR 2003-13789	20030822
CN 1678310	A	20051005	CN 2003-820093	20030822
JP 2006500398	T2	20060105	JP 2004-535140	20030822
ZA 2005001196	A	20050901	ZA 2005-1196	20050210
NO 2005001444	A	20050519	NO 2005-1444	20050318
PRIORITY APPLN. INFO.:			US 2002-405594P	P 20020824
			WO 2003-EP9329	W 20030822

OTHER SOURCE(S): MARPAT 140:264487

AB The invention discloses disorazole compds. which are used as medicaments, preferably in the treatment of tumors, especially in the case of drug resistance

and in metastasizing carcinoma. Possible uses thereof are not restricted to tumor diseases.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 3 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:149217 HCAPLUS

DOCUMENT NUMBER: 141:77736  
 TITLE: LSC measurements of the half-life of 40K  
 AUTHOR(S): Kossert, K.; **Gunther, E.**  
 CORPORATE SOURCE: Department 6.1, Physikalisch-Technische Bundesanstalt, Braunschweig, 38116, Germany  
 SOURCE: Applied Radiation and Isotopes (2004), 60(2-4), 459-464  
 CODEN: ARISEF; ISSN: 0969-8043  
 PUBLISHER: Elsevier Science B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Liquid scintillation counting techniques combined with the CIEMAT/NIST method have been applied to measure the specific activity of natural potassium salts. Samples have been prepared with three different scintillators. The individual atomic composition as well as the d. of the cocktails have been taken into account for the efficiency calcn. With the specific activity the half-life is calculated to be  $T_{1/2} = 1.248(3) + 109$  a. The result is in reasonable agreement with other measurement results provided the same isotopic concentration of 40K is used.  
 REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 4 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2004:149215 HCAPLUS  
 DOCUMENT NUMBER: 141:30008  
 TITLE: Ionization quenching in LSC  
 AUTHOR(S): Carles, Grau; **Gunther, E.**; Garcia, G.; Malonda, A. Grau  
 CORPORATE SOURCE: CIEMAT, Instituto de Estudios de la Energia, Madrid, 28040, Spain  
 SOURCE: Applied Radiation and Isotopes (2004), 60(2-4), 447-451  
 CODEN: ARISEF; ISSN: 0969-8043  
 PUBLISHER: Elsevier Science B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Ionization quench function  $Q(E)$  introduces an important correction in the CIEMAT/NIST tracing method. The authors present a detailed anal. of the equations used to compute the counting efficiency of  $^{55}\text{Fe}$ . The counting efficiency of this radionuclide is very sensitive to the shape and values of  $Q(E)$  for this method. The Birks equation and stopping power are not adequate to obtain low discrepancies between the exptl. and computed efficiencies. An empirical procedure to compute accurate  $Q(E)$  functions is also given.  
 REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 5 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2004:120730 HCAPLUS  
 DOCUMENT NUMBER: 140:157434  
 TITLE: Use of alkyl phosphocholines in combination with antitumor medicaments for the treatment of benign and malignant tumors  
 INVENTOR(S): Engel, Jorgen; **Gunther, Eckhard**; Sindermann, Herbert  
 PATENT ASSIGNEE(S): Zentaris GmbH, Germany  
 SOURCE: PCT Int. Appl., 21 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004012744	A1	20040212	WO 2003-EP8346	20030729
W: AU, BR, BY, CA, CN, CO, GE, HR, ID, IL, IN, IS, JP, KR, KZ, LT, LV, MK, MX, NO, NZ, PH, PL, RU, SG, UA, UZ, YU, ZA				
RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
CA 2493023	AA	20040212	CA 2003-2493023	20030729
AU 2003253350	A1	20040223	AU 2003-253350	20030729
BR 2003013048	A	20050614	BR 2003-13048	20030729
EP 1545553	A1	20050629	EP 2003-766336	20030729
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1671397	A	20050921	CN 2003-818101	20030729
JP 2005535688	T2	20051124	JP 2004-525354	20030729
US 2004097470	A1	20040520	US 2003-632187	20030730
CA 2436332	AA	20050131	CA 2003-2436332	20030731
ZA 2005000453	A	20050718	ZA 2005-453	20050118
NO 2005001040	A	20050225	NO 2005-1040	20050225
PRIORITY APPLN. INFO.:			US 2002-399615P	P 20020730
			WO 2003-EP8346	W 20030729

OTHER SOURCE(S): MARPAT 140:157434

AB The invention discloses the use of alkyl phosphocholines in combination with antitumor medicaments for treating benign and malignant tumor diseases in humans and mammals. The alkyl phosphocholines can be used in combination with one or a combination of several approved cytostatics. Compds. of the invention include e.g. perifosine.

L17 ANSWER 6 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:912847 HCAPLUS

DOCUMENT NUMBER: 139:395749

TITLE: Isolation and synthesis of decalactones from Penicillium species and methods for making pharmaceuticals there from

INVENTOR(S): Bringmann, Gerhard; Proksch, Peter; Edrada, Ru Angelie; Heubes, Markus; Gunther, Eckhard

PATENT ASSIGNEE(S): Biotecmarin GmbH, Germany

SOURCE: U.S. Pat. Appl. Publ., 8 pp.

CODEN: USXXCO

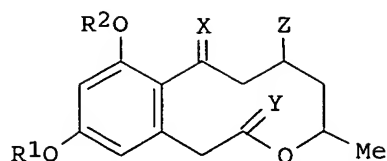
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003216354	A1	20031120	US 2002-143596	20020509
US 6872747	B2	20050329		
PRIORITY APPLN. INFO.:			US 2002-143596	20020509
OTHER SOURCE(S):			CASREACT 139:395749; MARPAT 139:395749	
GI				



I

AB A novel class of decalactones I [R1 = H, (un)branched C1-6-alkyl or C1-6-alkyl mono- or multisubstituted by C6-14-aryl, (un)branched carboxy(C1-18-alkyl), (un)branched (C1-6-alkoxy)carbonyl, (un)branched (C1-12-alkyl)carbonyl, C2-6-alkenyl, C2-6-alkynyl, (un)branched cyano(C1-18-alkyl), OCH2Ph, (9-fluorenylmethoxy)carbonyl (Fmoc), CPh3, 2-(4-pyridyl)ethoxycarbonyl (Pyoc), SiPh2Me (DPMS); R2 = R1; X = O, S, NOH, NOR4; Y = O, S; Z = H, OR3; R3 = R1; R4 = (un)branched C1-6-alkyl or C1-6-alkyl mono- or multisubstituted by C6-14-aryl, (un)branched carboxy(C1-18-alkyl), (un)branched (C1-6-alkoxy)carbonyl, (un)branched (C1-12-alkyl)carbonyl], and their enantiomers [R, S] or stereoisomers [(R,R), (R,S), (S,S)] or mixts. thereof, and a method for their isolation is disclosed. Thus, xestodecalactone A [(+)-I; R1 = R2 = H, X = Y = O, Z = H] was isolated from fungus of *Penicillium* sp. found on freshly collected samples of marine sponge *Xestospongia exigua*. A method for the synthesis of the decalactones I and the use of the decalactones in pharmaceutical compns. is also described. Thus, (±)-I [R1 = R2 = H, X = Y = O, Z = H] was prepared from 3,5-(HO)2C6H3CH2CO2Me and MeC(:O)(CH2)3CO2H via coupling of 3,5-(PhCH2O)2C6H3CH2CO2H with MeC(OH)(CH2)3CO2Me and intramol. acylation of 3,5-(PhCH2O)2C6H3CH2CO2CHM3(CH2)3CO2H, followed by hydrogenolytic debenzoylation. The antitumor activity of I (0.003 - 3.16 µg) was determined (no data).

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 7 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:414842 HCAPLUS

DOCUMENT NUMBER: 139:226932

TITLE: Evariquinone, isoemicellin, and stromemycin from a sponge derived strain of the fungus *Emericella varicolor*

AUTHOR(S): Bringmann, Gerhard; Lang, Gerhard; Steffens, Stefan; **Gunther, Eckhard**; Schaumann, Karsten

CORPORATE SOURCE: Institut fuer Organische Chemie der Universitaet, Wuerzburg, D-97074, Germany

SOURCE: Phytochemistry (Elsevier) (2003), 63(4), 437-443  
CODEN: PYTCAS; ISSN: 0031-9422

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB From a strain of the fungus *Emericella varicolor* derived from the marine sponge *Haliclona valliculata*, two new natural products, evariquinone and isoemicellin, were isolated after HPLC-UV, -MS, and -NMR studies of the extract and their structures were elucidated by mass spectrometry and NMR expts. Evariquinone showed antiproliferative activity towards KB and NCI-H460 cells at a concentration of 3.16 µg/mL. Furthermore, the fungus was found to produce the known metabolites stromemycin, shamixanthone, and 7-hydroxyemodin. Chemical degradation, NMR decoupling expts., and spin-system

simulation provided evidence for the double bonds in stromemycin to be all E-configured. ROESY expts. established the monosaccharide moiety to be glucose.

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 8 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:980623 HCAPLUS

DOCUMENT NUMBER: 139:75039

TITLE: Characterisation of ceramic breeder materials for the helium cooled pebble bed blanket

AUTHOR(S): Piazza, G.; Reimann, J.; Gunther, E.; Knitter, R.; Roux, N.; Lulewicz, J. D.

CORPORATE SOURCE: Institute for Nuclear and Energy Technologies, Forschungszentrum Karlsruhe, Karlsruhe, 76021, Germany

SOURCE: Journal of Nuclear Materials (2002), 307-311(Pt. A), 811-816

CODEN: JNUMAM; ISSN: 0022-3115

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In the European He cooled pebble bed (HCPB) blanket slightly hyperstoichiometric Li orthosilicate ( $\text{Li}_4\text{SiO}_4+\text{SiO}_2$ ) and Li metatitanate ( $\text{Li}_2\text{TiO}_3+\text{TiO}_2$ ) pebbles are considered as candidate ceramic breeder materials. Such ceramic breeder pebbles and pebble beds were studied in different types of expts. carried out at Forschungszentrum Karlsruhe. In longterm annealing expts. (96 days at  $970^\circ$  in  $\text{He}+0.1\% \text{H}_2$  atmosphere) the behavior of the pebbles under DEMO blanket relevant conditions was studied. Mech. uniaxial and triaxial compression tests at temps. up to  $\text{apprx.}850^\circ$  were performed to determine the mech. behavior of pebble beds as a function of temperature (stress-strain dependence, thermal creep behavior, friction coeffs.). Thermal conductivity measurements up to  $\text{apprx.}800^\circ$  were carried out with the aim to study the effect of creep on the pebble bed heat conduction. An overview of the exptl. activities on ceramic breeder materials is given.

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 9 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:589583 HCAPLUS

DOCUMENT NUMBER: 137:176626

TITLE: Probing dust around brown dwarfs. The naked LP 944-20 and the disk of Chamaeleon H $\alpha$  2

AUTHOR(S): Apai, D.; Pascucci, I.; Henning, Th.; Sterzik, M. F.; Klein, R.; Semenov, D.; Gunther, E.; Stecklum, B.

CORPORATE SOURCE: Astrophysikalisches Institut und Universitats-Sternwarte, Jena, D-07745, Germany

SOURCE: Astrophysical Journal (2002), 573(2, Pt. 2), L115-L117 CODEN: ASJOAB; ISSN: 0004-637X

PUBLISHER: University of Chicago Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We present the 1st mid-IR (MIR) detection of a field brown dwarf (BD) and the 1st ground-based MIR measurements of a disk around a young BD candidate. We prove the absence of warm dust surrounding the field BD LP 944-20. In the case of the young BD candidate Cha H $\alpha$  2, we find clear evidence for thermal dust emission from a disk. Surprisingly, the object does not exhibit any silicate feature as previously predicted. We show that the flat spectrum can be explained by an optically thick flat

dust disk.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 10 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:1269 HCAPLUS

DOCUMENT NUMBER: 136:209711

TITLE: What can we expect from the CIEMAT/NIST method?

AUTHOR(S): Gunther, E.

CORPORATE SOURCE: Physikalisch-Technische Bundesanstalt (PTB),  
Braunschweig, 38116, Germany

SOURCE: Applied Radiation and Isotopes (2002), 56(1-2),  
357-360

CODEN: ARISEF; ISSN: 0969-8043

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB During the last years the CIEMAT/NIST (C/N) method was widely used to determine activities of different radionuclides. The impression is given that the C/N method could be a universal method for all types of radionuclides. This paper shows under which conditions the C/N method can be used, where its limits are and which uncertainties can typically be achieved.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 11 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:1258 HCAPLUS

DOCUMENT NUMBER: 136:407005

TITLE: Determination of the 32P activity in angioplastic balloons by LSC

AUTHOR(S): Gunther, E.

CORPORATE SOURCE: Physikalisch-Technische Bundesanstalt (PTB),  
Braunschweig, 38116, Germany

SOURCE: Applied Radiation and Isotopes (2002), 56(1-2),  
291-293

CODEN: ARISEF; ISSN: 0969-8043

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The determination of the 32P activity in angioplastic balloons involves two problems: the extraction of 32P, which is covered with plastic foils, and the determination of the 33P impurity. At PTB the active balloons are destroyed by combustion in an oxygen stream. The active phosphorus is extracted quant. from the tube. The activities of 32P and 33P are determined by measurements performed over a period of one month or more by a subsequent data fit.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 12 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:906962 HCAPLUS

DOCUMENT NUMBER: 137:74215

TITLE: Genomic analysis of MIC genes in rhesus macaques

AUTHOR(S): Seo, J. W.; Walter, L.; Gunther, E.

CORPORATE SOURCE: Abteilung Immunogenetik, Georg-August-Universitat,  
Gottingen, D-37073, Germany

SOURCE: Tissue Antigens (2001), 58(3), 159-165

CODEN: TSANA2; ISSN: 0001-2815

PUBLISHER: Munksgaard International Publishers Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB MIC genes map to the major histocompatibility complex (MHC) and are distantly related to MHC class I genes. Recently, MICA/MICB-like genes have been described in nonhuman primates. In *Macaca mulatta*, three MICA/B-like genes could be identified: Mamu-MIC1, Mamu-MIC2, and Mamu-MIC3. We show here the isolation and characterization of rhesus macaque cosmid clones which carry the Mamu-MIC2 and Mamu-MIC3 genes. Neither the MIC2- and MIC3-coding sequences nor resp. flanking sequences can be aligned unambiguously to either the human HLA-MICA or -MICB subregions, although MIC2 was found at a similar distance to the BAT1 gene as known for MICB in human. Thus, the characteristics allowing for a classification of primate MIC genes as being of the MICA or MICB types appear to have evolved after the separation of humans and rhesus monkeys from a common ancestor. Furthermore, also Mamu-MICD-containing cosmids could be isolated. In contrast to Mamu-MIC2 and Mamu-MIC3, the Mamu-MICD gene and its flanking sequences are highly conserved and orthologous to the human MICD subregion.

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 13 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:894716 HCAPLUS

DOCUMENT NUMBER: 136:125154

TITLE: Behaviour of ceramic breeder materials in long time annealing experiments

AUTHOR(S): Piazza, G.; Reimann, J.; Gunther, E.; Knitter, R.; Roux, N.; Lulewicz, J. D.

CORPORATE SOURCE: IKET, Forschungszentrum Karlsruhe, Karlsruhe, D-76021, Germany

SOURCE: Fusion Engineering and Design (2001), 58-59, 653-659  
CODEN: FEDEEE; ISSN: 0920-3796

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In the development of the European Helium Cooled Pebble Bed (HCPB) blanket the reference material is slightly overstoichiometric lithium orthosilicate ( $\text{Li}_4\text{SiO}_4+\text{SiO}_2$ ) pebbles, fabricated by the melting-spraying method. Slightly overstoichiometric lithium metatitanate ( $\text{Li}_2\text{TiO}_3+\text{TiO}_2$ ) and lithium metazirconate ( $\text{Li}_2\text{ZrO}_3+\text{ZrO}_2$ ) pebbles, fabricated using a extrusion-spheronization-sintering process, are considered as alternative candidates for the ceramic breeder material. In order to compare the long-term behavior of the three materials at HCPB-blanket relevant temperature and atmospheric ( $\text{He}+0.1\% \text{H}_2$ ), a campaign of three long time annealing expts.

were carried out at Forschungszentrum Karlsruhe (FZK). Pebbles of each ceramic breeder material ( $\text{Li}_4\text{SiO}_4+\text{SiO}_2$  from FZK,  $\text{Li}_2\text{TiO}_3+\text{TiO}_2$  and  $\text{Li}_2\text{ZrO}_3+\text{ZrO}_2$  from CEA) were annealed for 96 days at 970 °C. During this period the change of the mech. characteristics, the microstructure, and the chemical composition of the pebbles was analyzed. After the end of the annealing experiment,

uniaxial compression tests of pebble beds were performed addnl. In the present paper the results from the second exptl. campaign are reported and discussed.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 14 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:415887 HCAPLUS

DOCUMENT NUMBER: 135:227218

TITLE: Syntheses of racemic and non-racemic silicon- and germanium-containing  $\alpha$ -amino acids of the

formula type  $\text{H}_2\text{NCH}(\text{CH}_2\text{ElR}_3)\text{COOH}$  (El=Si, Ge; R=organyl) and incorporation of D- $\text{H}_2\text{NCH}(\text{CH}_2\text{SiMe}_3)\text{COOH}$  and D- $\text{H}_2\text{NCH}(\text{CH}_2\text{GeMe}_3)\text{COOH}$  into biologically active decapeptides: a study on C/Si/Ge bioisosterism

AUTHOR(S): Merget, Marcus; Gunther, Kurt; Bernd, Michael; **Gunther, Eckhard**; Tacke, Reinhold

CORPORATE SOURCE: Institut für Anorganische Chemie, Universität Würzburg, Würzburg, D-97074, Germany

SOURCE: Journal of Organometallic Chemistry (2001), 628(2), 183-194  
CODEN: JORCAI; ISSN: 0022-328X

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:227218

AB Two novel efficient methods for the synthesis of racemic silicon- and germanium-containing  $\alpha$ -amino acids of the formula type  $\text{rac-H}_2\text{NCH}(\text{CH}_2\text{ElR}_3)\text{COOH}$  (El = Si, Ge; R = organyl), starting from 3,6-diethoxy-2,5-dihydropyrazine, have been developed. Racemic  $\alpha$ -amino acids synthesized:  $\text{rac-H}_2\text{NCH}(\text{CH}_2\text{SiMe}_3)\text{COOH}$  (rac-2),  $\text{rac-H}_2\text{NCH}(\text{CH}_2\text{GeMe}_3)\text{COOH}$  (rac-3),  $\text{rac-H}_2\text{NCH}(\text{CH}_2\text{SiMe}_2\text{Ph})\text{COOH}$  (rac-4),  $\text{rac-H}_2\text{NCH}(\text{CH}_2\text{GeMe}_2\text{Ph})\text{COOH}$  (rac-5), and  $\text{rac-H}_2\text{NCH}(\text{CH}_2\text{SiMe}_2\text{CH}:\text{CH}_2)\text{COOH}$  (rac-6). Preparative liquid-chromatog. resolution of rac-2 and rac-3 [CHIROBIOTIC T (glycopeptide Teicoplanin covalently linked to spherical silica gel) as the stationary phase] yielded the  $\alpha$ -amino acids (R)-2, (S)-2, (R)-3, and (S)-3. The (R)- and (S)-enantiomers of  $\beta$ -(trimethylsilyl)alanine [(R)- and (S)-2] and  $\beta$ -(trimethylgermyl)alanine [(R)- and (S)-3] are sila- and germa-analogs, resp., of the antipodes of the non-proteinogenic  $\alpha$ -amino acid  $\beta$ -tert-butylalanine [(S)- and (R)- $\text{H}_2\text{NCH}(\text{CH}_2\text{CMe}_3)\text{COOH}$ ; (S)- and (R)-1]. Starting from the N-Fmoc-protected C/Si/Ge-analogous (D-configuration)  $\alpha$ -amino acids (R)-1, (S)-2, and (S)-3, the C/Si/Ge-analogous decapeptides 7-9 [Ac-D-Nal1-4-C1-D-Phe2-D-Pal3-Ser4-N-Me-Tyr5-D-Hci6-Nle7-Arg8-Pro9-D-Me3El-Ala10-NH2 (7, El = C; 8, El = Si; 9, El = Ge)] were prepared by sequential solid-phase synthesis. The decapeptides 7-9 were studied in vitro in a functional assay using a recombinant cell line expressing the human GnRH receptor (agonist Triptorelin). Compds. 7-9 behaved as medium-potent GnRH antagonists, the antagonistic potencies of these three C/Si/Ge analogs being very similar.

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 15 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:278963 HCAPLUS

DOCUMENT NUMBER: 135:10626

TITLE: Standardisation and decay data of 177Lu and 188Re

AUTHOR(S): Schotzig, U.; Schrader, H.; Schonfeld, E.; **Gunther, E.**; Klein, R.

CORPORATE SOURCE: Physikalisch-Technische Bundesanstalt, Braunschweig, 38116, Germany

SOURCE: Applied Radiation and Isotopes (2001), 55(1), 89-96  
CODEN: ARISEF; ISSN: 0969-8043

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The activity values of 177Lu and 188Re standard sources were measured using the  $4\pi\beta$ - $\gamma$ -coincidence method and by liquid scintillation counting. The x- and gamma-ray emission probabilities per disintegration were determined by means of photon spectrometry with calibrated Ge and Si(Li) detectors and using the pertinent activity values. The half-lives were



measured with ionization chambers, yielding  $T_{1/2}(^{177}\text{Lu}) = 6.646(5)$  d and  $T_{1/2}(^{188}\text{Re}) = 0.70848(9)$  d.

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 16 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:132620 HCAPLUS

DOCUMENT NUMBER: 135:353252

TITLE: Comparative genomic aspects of rat, mouse and human MHC class I gene regions

AUTHOR(S): Gunther, E.; Walter, L.

CORPORATE SOURCE: Abteilung Immunogenetik, Georg-August-Universitat, Gottingen, D-37073, Germany

SOURCE: Cytogenetics and Cell Genetics (2000), 91(1-4), 107-112

CODEN: CGCGBR; ISSN: 0301-0171

PUBLISHER: S. Karger AG

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review with refs. In this review a particular aspect of the genomic structure of the major histocompatibility complex (MHC), the organization of MHC class I regions, will be discussed for the rat in comparison to mouse and human.

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 17 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:48557 HCAPLUS

DOCUMENT NUMBER: 134:196851

TITLE: Manufacturing and characterization of piezoceramic lead metaniobate  $\text{PbNb}_2\text{O}_6$

AUTHOR(S): Ray, S.; Gunther, E.; Ritzhaupt-Kleissl, H.-J.

CORPORATE SOURCE: Forschungszentrum Karlsruhe GmbH, Institut fur Materialforschung III, Karlsruhe, D-76021, Germany

SOURCE: Journal of Materials Science (2000), 35(24), 6221-6224

CODEN: JMTSAS; ISSN: 0022-2461

PUBLISHER: Kluwer Academic Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The synthesis of single-phase lead metaniobate  $\text{PbNb}_2\text{O}_6$  powders by a novel Thermal Two-Stage Process is described. Ceramic parts are produced from these powders by dry pressing and sintering. Following polarization, the piezoelec. properties of the specimens are measured. The piezoelec. material data of the specimens from this novel processing route are comparable with the values known from literature.

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 18 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:894792 HCAPLUS

DOCUMENT NUMBER: 134:141823

TITLE: New LHRH antagonists with enhanced biological activity: Preclinical and clinical results

AUTHOR(S): Kutscher, Bernhard; Bernd, Michael; Gunther, Eckhard; Deger, Wolfgang; Reissmann, Thomas; Beckers, Thomas; Deghenghi, Romano; Engel, Jurgen

CORPORATE SOURCE: Corporate Research, ASTA Medica AG, Frankfurt, D-60314, Germany

SOURCE: Peptides for the New Millennium, Proceedings of the

American Peptide Symposium, 16th, Minneapolis, MN, United States, June 26-July 1, 1999 (2000), Meeting Date 1999, 655-657. Editor(s): Fields, Gregg B.; Tam, James P.; Barany, George. Kluwer Academic Publishers: Dordrecht, Neth.  
CODEN: 69ATHX

DOCUMENT TYPE: Conference; General Review  
LANGUAGE: English

AB A brief review/discussion with 4 refs. on the title topic with focus on Cetrorelix, Antarelix, and D-26344 and their use in treating sex hormone-dependent tumors and nonmalignant conditions.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 19 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:883024 HCAPLUS

DOCUMENT NUMBER: 134:126130

TITLE: Molecular dynamics simulations of the binding of a GnRH agonist to a model GnRH receptor  
AUTHOR(S): ter Laak, A. M.; Kuhne, R.; Krause, G.; Polymeropoulos, E. E.; Kutscher, B.; Gunther, E.

CORPORATE SOURCE: Forschungsinstitut fur Molekulare Pharmakologie, Berlin, 10315, Germany

SOURCE: Molecular Modeling and Prediction of Bioactivity, [Proceedings of the European Symposium on Quantitative Structure-Activity Relationships: Molecular Modeling and Prediction of Bioactivity], 12th, Copenhagen, Denmark, Aug. 23-28, 1998 (2000), Meeting Date 1998, 397-398. Editor(s): Gundertofte, Klaus; Jorgensen, Flemming Steen. Kluwer Academic/Plenum Publishers: New York, N. Y.  
CODEN: 69ASO3

DOCUMENT TYPE: Conference  
LANGUAGE: English

AB Gonadotropin-releasing hormone (GnRH) is the naturally occurring agonist for the G-protein-coupled GnRH receptor. GnRH stimulates the pituitary gland to produce LH and FSH, and both GnRH agonists and antagonists are potentially useful in the treatment of hormone dependent ailments. The aim of the present modeling study is the generation of a 3D-model for the binding of GnRH agonists to the GnRH receptor model using a mol. dynamics protocol with carefully designed range distance restraint functions. At a second stage in the same mol. dynamics run, the possible conformational changes within the receptor after agonist binding are investigated by simulating hypothetical conformational changes of selected conserved amino acid side chains within the GnRH receptor.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 20 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:744589 HCAPLUS

DOCUMENT NUMBER: 134:49835

TITLE: Microstructure and piezoelectric properties of lead metaniobate PbNb2O6

AUTHOR(S): Ray, S.; Sauermann, Y.; Paul, F.; Gunther, E.; Ritzhaupt-Kleissl, H. -J.

CORPORATE SOURCE: Forschungszentrum Karlsruhe GmbH, Institut fur Materialforschung III, Germany

SOURCE: EUROMAT 99, Biannual Meeting of the Federation of European Materials Societies (FEMS), Munich, Germany,

Sept. 27-30, 1999 (2000), Meeting Date 1999, Volume  
13, 428-432. Editor(s): Grassie, K. Wiley-VCH Verlag  
GmbH: Weinheim, Germany.  
CODEN: 69AMNI

DOCUMENT TYPE: Conference  
LANGUAGE: English

AB In this contribution an overview is given of the influence of various  
processing parameters, sintering parameters in particular, on the  
development of the microstructure of piezoceramic samples made of lead  
metaniobate PbNb<sub>2</sub>O<sub>6</sub>. Also, the influence of the microstructure on the  
resulting piezoelec. properties of the material is discussed briefly.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 21 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:666761 HCAPLUS

DOCUMENT NUMBER: 133:256821

TITLE: Novel LHRH antagonists with improved solubility  
characteristics

INVENTOR(S): Bernd, Michael; Kutscher, Bernhard; Gunther,  
Eckhard; Romeis, Peter; Reissmann, Thomas;  
Beckers, Thomas

PATENT ASSIGNEE(S): Asta Medica A.-G., Germany

SOURCE: PCT Int. Appl., 30 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000055190	A1	20000921	WO 2000-EP2165	20000311
W: AU, BG, BR, BY, CA, CN, CZ, EE, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LT, LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, UZ, YU, ZA, AM, AZ, MD, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
DE 19911771	A1	20000928	DE 1999-19911771	19990317
CA 2381461	AA	20000921	CA 2000-2381461	20000311
BR 2000009472	A	20011127	BR 2000-9472	20000311
EP 1163264	A1	20011219	EP 2000-910816	20000311
EP 1163264	B1	20040922		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 200103339	T2	20020422	TR 2001-200103339	20000311
JP 2002543045	T2	20021217	JP 2000-605616	20000311
AU 759442	B2	20030417	AU 2000-32887	20000311
NZ 514830	A	20030530	NZ 2000-514830	20000311
RU 2227145	C2	20040420	RU 2001-128232	20000311
AT 277077	E	20041015	AT 2000-910816	20000311
PT 1163264	T	20041231	PT 2000-910816	20000311
ES 2225103	T3	20050316	ES 2000-910816	20000311
NO 2001004486	A	20011102	NO 2001-4486	20010914
ZA 2001007753	A	20020513	ZA 2001-7753	20010919
BG 106008	A	20020628	BG 2001-106008	20011011
HK 1045531	A1	20050520	HK 2002-107028	20020926
US 2004266695	A1	20041230	US 2003-671573	20030929
PRIORITY APPLN. INFO.:			DE 1999-19911771	A 19990317
			WO 2000-EP2165	W 20000311

US 2000-525007

A3 20000314

OTHER SOURCE(S): MARPAT 133:256821

AB The invention relates to peptides which contain N-methylated amino acid building blocks and are provided with improved water solubility. Medicaments containing the inventive peptides can be used for the treatment of hormone-dependent tumors and hormone-influenced, non-malignant diseases.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 22 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:509345 HCAPLUS

DOCUMENT NUMBER: 133:157847

TITLE: Structural investigations on the oxidenitrides SrTaO<sub>2</sub>N, CaTaO<sub>2</sub>N and LaTaON<sub>2</sub> by neutron and x-ray powder diffraction

AUTHOR(S): Gunther, E.; Hagenmayer, R.; Jansen, M.

CORPORATE SOURCE: Max-Planck-Inst. Festkörperforschung, Stuttgart, D-70569, Germany

SOURCE: Zeitschrift fuer Anorganische und Allgemeine Chemie (2000), 626(7), 1519-1525  
CODEN: ZAACAB; ISSN: 0044-2313

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: German

AB The crystal structures of the perovskite related oxidenitrides SrTaO<sub>2</sub>N, LaTaON<sub>2</sub>, and CaTaO<sub>2</sub>N were determined with special regard to the structures of the resp. anionic partial structure. The structure refinements were performed by individual Rietveld analyses of both x-ray and neutron powder diffractograms and in addition by joint refinements to confirm the results. Both refinement methods yield consistent structure solns. At least the 1st 2 compds. have fully ordered anionic sublattices. The crystal structure of SrTaO<sub>2</sub>N was solved in the space group I4/mcm (a = 5.7049(3), c = 8.0499(5) Å, R<sub>p</sub> = 0.0706, R<sub>wp</sub> = 0.0904, reflections: 70 (neutrons)/36 (x-ray), R(F<sub>2</sub>)(n) = 0.147, R(F<sub>2</sub>)(X) = 0.0952), with an ordered anionic partial structure. LaTaON<sub>2</sub> crystallizes monoclinic (C2/m, a = 8.0922(3), b = 8.0603(2), c = 5.7118(2) Å, β = 134.815(1)°, R<sub>p</sub> = 0.0592, R<sub>wp</sub> = 0.0766, reflections: 235(n)/113(X), R(F<sub>2</sub>)(n) = 0.0944, R(F<sub>2</sub>)(X) = 0.165) and also shows a totally ordered distribution of the anions. In the case of CaTaO<sub>2</sub>N (Pnma, a = 5.6239(3), b = 7.8954(4), c = 5.5473(3) Å, R<sub>p</sub> = 0.0503, R<sub>wp</sub> = 0.0656, reflections 206(n)/110(X), R(F<sub>2</sub>)(n) = 0.0985, R(F<sub>2</sub>)(X) = 0.0405) slightly unbalanced displacement parameters (neutron data, ordered O/N distribution model) hint at a partial exchange of O and N.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 23 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:318656 HCAPLUS

DOCUMENT NUMBER: 133:28908

TITLE: Tissue transglutaminase in the small intestine of the mouse as a marker for apoptotic cells. Colocalization with DNA fragmentation

AUTHOR(S): Aschoff, A. P.; Gunther, E.; Jirikowski, G. F.

CORPORATE SOURCE: Department of Anatomy II, FSU-Jena, Jena, 07743, Germany

SOURCE: Histochemistry and Cell Biology (2000), 113(4), 313-317

CODEN: HCBIFP; ISSN: 0948-6143

PUBLISHER: Springer-Verlag

DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Besides the morphol. changes in cells undergoing apoptosis, such as chromatin condensation and cell shrinkage, histol. demonstration of DNA fragmentation by in situ end labeling (ISEL) has been widely used for the demonstration of apoptotic cells in tissue sections. Although DNA fragmentation can be demonstrated in apoptotic cells and apoptotic bodies in most cases, there is no clear correlation of ISEL staining with apoptosis. It has often been demonstrated that, in many morphol. intact cells, nuclei with fragmented DNA can be found. Thus staining with ISEL for the detection of apoptosis is useful only in connection with other markers for apoptosis as, for example, characteristic morphol. changes. Here we show that tissue transglutaminase protein is unequivocally expressed in apoptotic enterocytes as shown by DNA fragmentation and morphol. Tissue transglutaminase is not expressed in enterocytes with healthy morphol., although DNA fragmentation can be demonstrated in these cells. Thus the immunohistochem. demonstration of tissue transglutaminase may serve as a simple marker for apoptotic epithelial cells in tissue sections.

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 24 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:292155 HCAPLUS

DOCUMENT NUMBER: 133:115600

TITLE: Report on rat chromosome 20

AUTHOR(S): Butcher, G.; Gunther, E.; Gill, T. J., III;  
Kunz, H. W.; Natori, T.

CORPORATE SOURCE: Immunology Department, The Babraham Institute,  
Cambridge, CB2 4AT, UK

SOURCE: Journal of Experimental Animal Science (1999),  
40(1-3), 143-153

CODEN: JEXSEU; ISSN: 0939-8600

PUBLISHER: Urban & Fischer Verlag

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review with 147 refs. compiling the 120 genes, 4 QTL, and about 125 DNA markers that have been mapped to rat chromosome 20. Several recent reports of maps are available that are based mainly on microsatellite markers.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 25 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:292142 HCAPLUS

DOCUMENT NUMBER: 133:115587

TITLE: Report on rat chromosome 7

AUTHOR(S): Gunther, E.; Levan, G.

CORPORATE SOURCE: Division of Immunogenetics, University of Gottingen,  
Gottingen, D - 37073, Germany

SOURCE: Journal of Experimental Animal Science (1999),  
40(1-3), 63-68

CODEN: JEXSEU; ISSN: 0939-8600

PUBLISHER: Urban & Fischer Verlag

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review with 41 refs. A compilation of the genes mapped to rat chromosome 7 is provided, as well as a cytogenetic map, linkage maps, and framework markers.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS

## RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 26 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:281531 HCAPLUS

DOCUMENT NUMBER: 132:304251

TITLE: Proceedings of the International Workshop on the  
Impact of Rat Genome Mapping on Biomedical Research,  
held 4-6 October 1998, in Lower Saxony, Germany. [In:  
J. Exp. Anim. Sci., 1999; 40(1-3)]

AUTHOR(S): **Gunther, E.**; Levan, G.; Jacob, H.; Hedrich,  
H. J.; Editors

CORPORATE SOURCE: Germany

SOURCE: (1999) Publisher: (Urban & Fischer: Jena, Germany),  
164 pp.

DOCUMENT TYPE: Book

LANGUAGE: English

AB Unavailable

L17 ANSWER 27 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:193472 HCAPLUS

DOCUMENT NUMBER: 132:268556

TITLE: Wet chemical methods for preparation of yttrium barium  
copper oxide (YBCO) and bismuth strontium calcium  
copper oxide (BSCCO) ceramic superconductors

AUTHOR(S): Binder, J. R.; **Gunther, E.**; Wedemeyer, H.;  
Ritzhaupt-Kleissl, H.-J.; Hausselt, J. H.

CORPORATE SOURCE: Forschungszentrum Karlsruhe GmbH, Institut fur  
Materialforschung III, Germany

SOURCE: Werkstoffwoche '98, Band VII: Symposium 9, Keramik;  
Symposium 14, Simulation Keramik, Munich, Sept., 1998  
(1999), Meeting Date 1998, 175-180. Editor(s):  
Heinrich, Juergen. Wiley-VCH Verlag GmbH: Weinheim,  
Germany.

CODEN: 68SUAA

DOCUMENT TYPE: Conference; General Review

LANGUAGE: German

AB A review with 9 refs. is given on manufacturing high-performance functional  
ceramics with uniform dopant distribution, shortened total time, and  
reduced sintering temperature Thin-film YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-x</sub> (YBCO) superconductor on  
monocryst. SrTiO<sub>3</sub> substrate can be prepared by a sol-gel method.  
Fine-scaled Pb-doped Bi<sub>2</sub>Sr<sub>2</sub>Ca<sub>2</sub>Cu<sub>3</sub>O<sub>10+x</sub> (BSCCO) superconductor powders can  
be prepared by a thermal two-stage procedure. Powders obtained thereby show  
excellent bulk material properties with good consolidation.

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 28 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:192263 HCAPLUS

DOCUMENT NUMBER: 132:213777

TITLE: Standardization of <sup>237</sup>Np by the CIEMAT/NIST LSC tracer  
method

AUTHOR(S): **Gunther, E.**

CORPORATE SOURCE: Physikalisch-Technische Bundesanstalt (PTB),  
Braunschweig, 38116, Germany

SOURCE: Applied Radiation and Isotopes (2000), 52(3), 471-474  
CODEN: ARISEF; ISSN: 0969-8043

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The standardization of <sup>237</sup>Np presents some difficulties: several groups of

alpha, beta and gamma radiation, chemical problems with the daughter nuclide <sup>233</sup>Pa, an incomplete radioactive equilibrium after sample preparation, and high conversion of some gamma transitions. To solve the chemical problems, a sample composition involving the Ultima Gold AB scintillator and a high concentration

of HCl was used. Standardization by the CIEMAT/NIST method using the <sup>3</sup>H tracer nuclide and by pulse shape discrimination is described. The results agree within 0.1% with those obtained by two other methods.

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 29 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:754855 HCAPLUS

DOCUMENT NUMBER: 134:96034

TITLE: Major histocompatibility complex-linked MIC genes in rhesus macaques and other primates

AUTHOR(S): Seo, J.-W.; Bontrop, R.; Walter, L.; Gunther, E.

CORPORATE SOURCE: Abteilung Immunogenetik, Georg-August-Universitat Gottingen, Gottingen, D-37037, Germany

SOURCE: Immunogenetics (1999), 50(5/6), 358-362

CODEN: IMNGBK; ISSN: 0093-7711

PUBLISHER: Springer-Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A group of class I genes has been identified in the human major histocompatibility complex (MHC), the HLA complex, that exhibit an organization similar to class Ia genes, but the gene products are only about 15-35% identical compared with various domains of class Ia mols. These novel genes, designated MIC or PERB11 occur in several copies, MICA (PERB11.1) to MICE (PERB11.5). To facilitate use of animal models, we have started to examine MIC genes in nonhuman primates. Here we clone, characterize and sequence MICA/B-like genes from *Macaca mulatta*, *Papio hamadryas* and *Ateles fusciceps*. Our results presented here confirm and extend the recent publication of primate MIC gene sequences (Steinle et al. 1998), and contribute to the delineation of their evolution. We found that MIC genes of *M. mulatta* and *P. hamadryas* are not orthologs of either human MICA or MICB, but these MIC genes appear to be derived from the same MIC ancestor gene which duplicated and diversified in the various primate species.

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 30 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:641376 HCAPLUS

DOCUMENT NUMBER: 132:10068

TITLE: M protein of a *Streptococcus dysgalactiae* human wound isolate shows multiple binding to different plasma proteins and shares epitopes with keratin and human cartilage

AUTHOR(S): Geyer, A.; Roth, A.; Vettermann, S.; Gunther, E.; Groh, A.; Straube, E.; Schmidt, K.-H.

CORPORATE SOURCE: Institute of Medical Microbiology, Hospital of the Friedrich-Schiller-University, Jena, D-07740, Germany

SOURCE: FEMS Immunology and Medical Microbiology (1999), 26(1), 11-24

CODEN: FIMIEV; ISSN: 0928-8244

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Besides group A (GAS), Lancefield group C  $\beta$ -hemolytic streptococci (GCS) have been implicated as a causative agent in outbreaks of purulent pharyngitis. In this study we have investigated a class CI M protein of a *Streptococcus dysgalactiae* human wound isolate designated MC. MC shares similar properties with M proteins of GAS. It contributes to the virulence of the investigated GCS strain as revealed by in vivo phagocytosis in chicken embryos. Further, MC showed multiple binding to the human plasma proteins fibrinogen, albumin, plasminogen, IgA and all subclasses of IgG. Until now, an M protein, especially from a group C strain, with such a multiple binding behavior has not been described. Immunoblot expts. with 150 patient sera, having a rheumatoid factor titer > 1:256, revealed that 26% of these sera showed serol. cross-reactivity between a 68-kDa cartilage protein and the N-terminal part of MC. Only 8% of the sera of healthy patients showed this property. In addition, MC also cross-reacted with antibodies recognizing epidermal keratins. The cross-reacting 68-kDa protein from cartilage was different from human serum albumin, but was recognized with anti-vimentin immune serum. The MC was cloned and the gene sequenced. By using PCR, recombinant gene fragments encoding characteristic peptide fragments of MC were expressed in *Escherichia coli*. The peptides were used to map the binding sites for plasma proteins and to locate the cross-reacting epitopes on the MC mol. In consequence, sequence alignments revealed that MC shared homologous regions with vimentin and different keratins. Our data, obtained with MC, suggest that not only infections with GAS but also infections with GCS and possibly GGS (the latter species can also produce class CI M-like proteins) may be responsible for the formation of streptococcal-associated sequel diseases.

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 31 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:572216 HCAPLUS

DOCUMENT NUMBER: 131:272102

TITLE: A practical synthesis of benzyl  $\alpha$ - and allyl  $\beta$ -D-glucopyranosides regioselectively substituted with (CH<sub>2</sub>)<sub>3</sub>OH groups. Stereocontrolled  $\beta$ -galactosidation by cation  $\pi$ -interaction

AUTHOR(S): Neda, Ion; Sakhaei, Peyman; Wassmann, Anke; Niemeyer, Ulf; Gunther, Eckhard; Engel, Jurgen

CORPORATE SOURCE: Institut Anorganische Analytische Chemie, Technische Univ. Braunschweig, Braunschweig, D-38023, Germany

SOURCE: Synthesis (1999), (9), 1625-1632

CODEN: SYNTBF; ISSN: 0039-7881

PUBLISHER: Georg Thieme Verlag

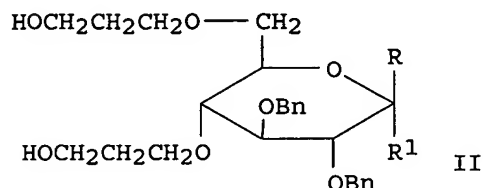
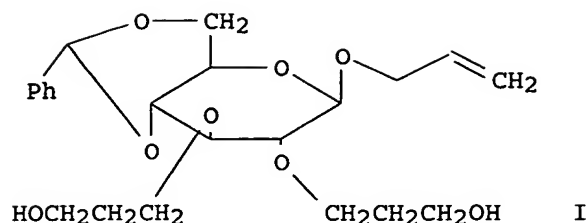
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 131:272102

GI





AB Efficient synthesis of the 2,3- or 4,6-di-O-hydroxypropyl-functionalized glucose derivs. I and II (R = allyloxy, R1 = H; R = H, R1 = PhCH2O) is presented. These compds. represent potential precursors for the synthesis of multi-antennary oligosaccharides. A new method was developed for the  $\beta$ -stereoselective galactosylation using galactosyl difluorophosphate as galactosyl donor and tetra-O-propylated cone-calix[4]arene as stabilizer for the oxo-carbenium ion. The latter compound is intended to serve (via immobilization on solid phase and subsequent deprotection) as affinity ligand in the isolation of tumor cell lectins via affinity chromatog.

REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 32 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:470418 HCAPLUS

DOCUMENT NUMBER: 131:232261

TITLE: Production of piezoceramic powders by the thermal two-stage process

AUTHOR(S): Weddigen, A.; Hennige, V. D.; Gunther, E.; Ritzhaupt-Kleissl, H.-J.

CORPORATE SOURCE: Forschungszentrum Karlsruhe, Institut fur Material forschung III, Karlsruhe, 76021, Germany

SOURCE: Journal of Materials Science (1999), 34(14), 3461-3465  
CODEN: JMTSAS; ISSN: 0022-2461

PUBLISHER: Kluwer Academic Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The present paper describes the production of lead zirconate titanate (PZT) with different additives and of lead metaniobate (PN) by means of the Thermal Two-Stage Process. This process, especially developed for the synthesis

of multicomponent ceramic powders is characterized by the following: the starting constituents are liquid metalorg. precursors, such as alcoholates or acetates, which are converted to a homogeneous, multicomponent ceramic powder by spray drying the liquid precursors, resulting in an organic granulate, which is then followed by the thermal conversion of this organic

powder into the final ceramic material. The resulting ceramic powder shows favorable properties with respect to homogeneity and further processing, e.g. pressing and sintering of compacts. The efficiency of the process will be demonstrated by the characterization of the piezoelec. properties of the sintered compacts.

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 33 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:362795 HCAPLUS

DOCUMENT NUMBER: 131:180515

TITLE: Sequence analysis of the genomic interval between the Rps18 and RT1-A genes in the RT1u haplotype

AUTHOR(S): Walter, L.; Gunther, E.

CORPORATE SOURCE: Division of Immunogenetics, University of Gottingen, Gottingen, 37073, Germany

SOURCE: Transplantation Proceedings (1999), 31(3), 1513-1514  
CODEN: TRPPA8; ISSN: 0041-1345

PUBLISHER: Elsevier Science Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The authors sequence and map the genomic interval between the rat genes Rps18 and RT1-A of the MHC RT1u haplotype.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 34 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:349427 HCAPLUS

DOCUMENT NUMBER: 131:64146

TITLE: Standardization and decay data of  $^{153}\text{Sm}$

AUTHOR(S): Schotzig, U.; Schonfeld, E.; Gunther, E.; Klein, R.; Schrader, H.

CORPORATE SOURCE: Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, D-38116, Germany

SOURCE: Applied Radiation and Isotopes (1999), 51(2), 169-175  
CODEN: ARISEF; ISSN: 0969-8043

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The activity concentration of a  $^{153}\text{Sm}$  solution was determined by  $4\pi\beta\text{-}\gamma$  coincidence measurements and by liquid scintillation counting (LSC). Both methods yielded results which differ by only 0.1%, the relative standard uncertainty being 0.1 and 0.2%, resp. X-ray and gamma-ray emission probabilities of several transitions were measured; they were used to calculate beta transition probabilities. The emission probabilities of the 69.7 and the 103.2 keV gamma rays were found to be  $0.0465 \pm 0.0005$  and  $0.2923 \pm 0.0018$ , resp.; and the half-life was found to be  $(46.274 \pm 0.007)$  h.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 35 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:244571 HCAPLUS

DOCUMENT NUMBER: 130:276778

TITLE: Methods of modulating serine/threonine protein kinase function with 5-azaquinoxaline-based compounds, compound preparation, and therapeutic use

INVENTOR(S): McMahon, Gerald; Kutscher, Bernhard; Gunther, Eckhard; App, Harald

PATENT ASSIGNEE(S): Asta Medica A.-G., Germany

SOURCE: PCT Int. Appl., 80 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9917759	A2	19990415	WO 1998-US20910	19981005
WO 9917759	A3	20000106		
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
ZA 9808961	A	19991004	ZA 1998-8961	19981001
CA 2306257	AA	19990415	CA 1998-2306257	19981005
AU 9895141	A1	19990427	AU 1998-95141	19981005
AU 757585	B2	20030227		
EP 1028729	A2	20000823	EP 1998-948606	19981005
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, RO			
BR 9814814	A	20001003	BR 1998-14814	19981005
TR 200000906	T2	20001121	TR 2000-200000906	19981005
US 6180631	B1	20010130	US 1998-166723	19981005
JP 2001518496	T2	20011016	JP 2000-514630	19981005
TR 200100385	T2	20020621	TR 2001-200100385	19981005
NZ 503431	A	20020726	NZ 1998-503431	19981005
RU 2223753	C2	20040220	RU 2000-111434	19981005
MX 200003255	A	20001110	MX 2000-3255	20000403
NO 2000001748	A	20000405	NO 2000-1748	20000405
BG 104392	A	20001229	BG 2000-104392	20000428
US 6727252	B1	20040427	US 2000-688199	20001016
HK 1031836	A1	20050401	HK 2001-102529	20010410
PRIORITY APPLN. INFO.:			US 1997-61123P	P 19971006
			US 1998-166723	A3 19981005
			WO 1998-US20910	W 19981005

OTHER SOURCE(S): MARPAT 130:276778

AB Methods are provided for modulating the function of serine/threonine protein kinases with 5-azaquinoxaline-based compds. The methods incorporate cells that express a serine/threonine protein kinase, e.g. RAF. In addition, methods are described for preventing and treating serine/threonine protein kinase-related abnormal conditions (e.g. cancer) in organisms with a compound identified by the invention. Furthermore, the invention pertains to 5-azaquinoxaline compds., their preparation, and pharmaceutical compns. comprising them.

L17 ANSWER 36 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:64168 HCAPLUS

DOCUMENT NUMBER: 130:279968

TITLE: Heterogeneous patterns of constitutive and heat shock induced expression of HLA-linked HSP70-1 and HSP70-2 heat shock genes in human melanoma cell lines

AUTHOR(S): Dressel, R.; Johnson, J. P.; Gunther, E.

CORPORATE SOURCE: Division of Immunogenetics, University of Gottingen, Gottingen, D-37073, Germany

SOURCE: Melanoma Research (1998), 8(6), 482-492  
CODEN: MREEEH; ISSN: 0960-8931  
PUBLISHER: Lippincott Williams & Wilkins  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The heat shock response, which is characterized by the induction of heat shock proteins, is known to affect the ability of tumor cells to cope with potentially adverse conditions such as hypoxia, glucose starvation and cytotoxic immune reactions. To assess the heat shock response of melanoma cells, spontaneous and heat shock induced expression of heat shock proteins was analyzed in a panel of 17 human melanoma cell lines. Constitutive expression of HSP27, HSP70, HSC70, HSP90 $\alpha\beta$  and GRP94 proteins was found in all the melanoma cell lines, and HSP70 and HSC70 were also induced by heat shock. The major heat inducible HLA-linked HSP70-1 and HSP70-2 genes were analyzed at the mRNA level. Basal expression and inducibility varied between the different melanoma cell lines. In addition, in situ hybridization demonstrated heterogeneous expression of these genes among single cells of a given cell line. In general, each melanoma cell line appears to exhibit an individual type of HSP70 expression that might reflect selection during tumor progression and therapy.

REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 37 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:771850 HCAPLUS  
DOCUMENT NUMBER: 130:164920  
TITLE: Intercomparisons 1996 - 1998: Uranium, 210Pb, 3H, 14C and thorium in urine  
AUTHOR(S): Gunther, E.; Hartmann, M.; Naurmann, M.  
CORPORATE SOURCE: Physikalisch-Technische Bundesanstalt, Braunschweig, Germany  
SOURCE: Fortschritte im Strahlenschutz (1998), FS-98-98-T(Nichtionisierende Strahlung mit ihr Leben in Arbeit und Umwelt, Band I), 352-357  
CODEN: FSTRER; ISSN: 1013-4506  
PUBLISHER: Verlag TUV Rheinland GmbH  
DOCUMENT TYPE: Journal; General Review  
LANGUAGE: German

AB A review with 10 refs. The working group "Incorporation Monitoring (AKI)" of the German-Swiss Radiation protection Association (FS) has performed interlab. comparisons of radionuclides in urine for many years. Since 1997, the intercomparisons have been carried out by the Bundesamt für Strahlenschutz (BfS) in collaboration with the Physikalisch-Technische Bundesanstalt (PTB). The results of intercomparisons of uranium, lead-210 (both in 1996), tritium (1997), thorium (1998) und carbon-14 (1998) in urine will be presented here.

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 38 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:483041 HCAPLUS  
DOCUMENT NUMBER: 129:183548  
TITLE: International comparison of measurements of the specific activity of tritiated water  
AUTHOR(S): Makepeace, J.; Altitzoglou, T.; Cassette, P.; Dryak, P.; Gunther, E.; Verrezen, F.; Broda, R.; Simpson, B.; Unterweger, M.  
CORPORATE SOURCE: NPL, Teddington, TW11 0LW, UK  
SOURCE: Applied Radiation and Isotopes (1998), 49(9-11),

1411-1416

CODEN: ARISEF; ISSN: 0969-8043

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An international comparison of measurements of the specific activity of tritiated H<sub>2</sub>O was carried out under the auspices of the ICRM Radionuclide Techniques Working Group. The comparison, in which nine labs. participated, involved the measurement of tritiated H<sub>2</sub>O samples of unknown specific activity at up to three different activity levels. The results of the comparison are reported, together with information on the measurement techniques employed and the measurement uncertainties.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 39 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:483040 HCAPLUS

DOCUMENT NUMBER: 129:183547

TITLE: Comparison of activity concentration measurement of <sup>63</sup>Ni and <sup>55</sup>Fe in the framework of the EUROMET 297 project

AUTHOR(S): Cassette, P.; Altzitzoglou, T.; Broda, R.; Colle, R.; Dryak, P.; De Felice, P.; Gunther, E.; Arcos, J. M. Los; Ratel, G.; Simpson, B.; Verrezen, F.

CORPORATE SOURCE: BNM-LPRI, CEA/DAMRI, Gif-sur-yvette, 91193, Fr.

SOURCE: Applied Radiation and Isotopes (1998), 49(9-11), 1403-1410

CODEN: ARISEF; ISSN: 0969-8043

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Eleven labs. participated in an intercomparison of activity concentration measurements using liquid scintillation counting (LSC) for the standardization of <sup>63</sup>Ni and <sup>55</sup>Fe in the frame of the EUROMET project Number 297 and under the coordination of LPRI. The purpose of this action was to compare the main LSC activity concentration measurement methods currently used in radioactive metrol., and to exchange models and ideas on LSC. This paper presents a summary of the results reported by the participant labs. and an overview of the measurement methods used.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 40 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:482976 HCAPLUS

DOCUMENT NUMBER: 129:183534

TITLE: Standardization of the EC nuclides <sup>55</sup>Fe and <sup>65</sup>Zn with the CIEMAT/NIST LSC tracer method

AUTHOR(S): Gunther, E.

CORPORATE SOURCE: Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, 38116, Germany

SOURCE: Applied Radiation and Isotopes (1998), 49(9-11), 1055-1060

CODEN: ARISEF; ISSN: 0969-8043

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A study is made of the standardization of <sup>55</sup>Fe and <sup>65</sup>Zn under different exptl. and theor. conditions. Sample composition, tracer nuclide, ionization quench approxns., kB values and approxns. for the average L Auger electron

energy, were varied to find out the optimum conditions. A standardization of <sup>55</sup>Fe and <sup>65</sup>Zn is possible with a relative standard uncertainty of .apprx.0.5% using <sup>54</sup>Mn as a tracer. However, the expts. with <sup>3</sup>H as a tracer show that the EC. decay model and the LSC theory which are included in the CIEMAT/NIST programs are not fully satisfactory for these two EC radionuclides.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 41 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:64556 HCAPLUS

DOCUMENT NUMBER: 128:131356

TITLE: Development of ceramic micro heat exchanger

AUTHOR(S): Knitter, R.; Gunther, E.

CORPORATE SOURCE: institut fur Materialforschung III, Forschungszentrum Karlsruhe GmbH, Karlsruhe, D-76201, Germany

SOURCE: Neue Werkstoffkonzepte, Symposium 9, Werkstoffwoche '96, Stuttgart, 1996 (1997), Meeting Date 1996, 221-226. Editor(s): Schmidt, H.; Singer, R. F. DGM Informationsgesellschaft: Oberursel, Germany. CODEN: 650AAB

DOCUMENT TYPE: Conference

LANGUAGE: German

AB Two processes: (i) foil casting and stamping and (ii) slip casting on pyrolyzed filaments for the manufacture of the title heat exchanger are described, and the features of the heat exchangers prepared by these 2 processes are compared.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 42 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:3638 HCAPLUS

DOCUMENT NUMBER: 128:125147

TITLE: Studies on streptococcal NAD-glycohydrolase: copurification of streptodornase A

AUTHOR(S): Gerlach, D.; Ozegowski, J. H.; Gunther, E.; Vettermann, S.; Kohler, W.

CORPORATE SOURCE: Inst. Experimentelle Mikrobiol., Friedrich-Schiller-Universitaet Jena, Jena, D-07745, Germany

SOURCE: Advances in Experimental Medicine and Biology (1997), 418(Streptococci and the Host), 601-603 CODEN: AEMBAP; ISSN: 0065-2598

PUBLISHER: Plenum Publishing Corp.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A method for the rapid isolation of NAD glycohydrolase is described. The method gave a yield of .apprx.30% with a 968-fold purification. In addition, a method for the first purification of streptodornase A, one of the 4 known streptococcal DNases, is described.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 43 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:59394 HCAPLUS

DOCUMENT NUMBER: 122:99055

TITLE: Purification and characterization of streptolysin O secreted by Streptococcus equisimilis (group C)

AUTHOR(S): Gerlach, D.; Koehler, W.; Gunther, E.; Mann, K.

CORPORATE SOURCE: Institute of Experimental Microbiology, Jena, D-07745,

Germany  
 SOURCE: Zentralblatt fuer Bakteriologie, Supplement (1994),  
 24(Bacterial Protein Toxins), 341-2  
 CODEN: ZBASE2; ISSN: 0941-018X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Streptolysin O (SLO) was purified from culture supernatants of group C streptococci. The final product was either the complete mol. (SLOn, isoelec. point 6.0) with the N-terminal sequence (Asp)-Ser-Asn-Lys-Gln-Asn-Thr-Ala-Asn-Thr-Glu-Thr- or a large fragment (SLOf, isoelec. point 7.3) with the N-terminal sequence Ala-Pro-Lys-Glu-Met-Pro-Leu-Glu-Ser-Ala-Glu-Lys-Glu-Glu-Lys- corresponding to residues 79 to 93 of a DNA-derived sequence.

L17 ANSWER 44 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:639591 HCAPLUS  
 DOCUMENT NUMBER: 121:239591  
 TITLE: Standardization and decay data of  $^{68}\text{Ge}/^{68}\text{Ga}$   
 AUTHOR(S): Schonfeld, E.; Schotzig, U.; **Gunther, E.**;  
 Schrader, H.  
 CORPORATE SOURCE: Physikalisch-Technische Bundesanstalt, Bundesallee,  
 D-38116, Germany  
 SOURCE: Applied Radiation and Isotopes (1994), 45(9), 955-61  
 CODEN: ARISEF; ISSN: 0883-2889  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A gamma and an x-ray spectrometer,  $4\pi\beta\text{-}\gamma$ -coincidence equipment, liquid-scintillation counting (LSC) equipment and a calibrated ionization chamber (IC) have been used to determine the decay scheme parameters of  $^{68}\text{Ga}$  and the specific activity of a  $^{68}\text{Ge}/^{68}\text{Ga}$  solution. The transition probability of the positron branch and the EC branch to the ground state of  $^{68}\text{Zn}$ , b1 and e1, the corresponding branches to the 1077 keV level of  $^{68}\text{Zn}$ , b2 and e2, the total emission probability of annihilation radiation from the  $^{68}\text{Ga}$  decay, pann, and the gamma-ray emission probabilities of the quanta corresponding to the 1077 keV transition (p1077) and to some weak transitions were redetd. The results are b1 =  $0.8785 \pm 0.0012$ , e1 =  $0.0892 \pm 0.0012$ , b2 =  $0.0129 \pm 0.004$ , e2 =  $0.0193 \pm 0.0004$ , pann =  $1.7829 \pm 0.0022$ , p1077 =  $0.0322 \pm 0.0003$ . The specific activity of a  $^{68}\text{Ge}/^{68}\text{Ga}$  solution was determined with a relative uncertainty of 1% ( $1\sigma$ ) using  $4\pi\beta\text{-}\gamma$  coincidence, LSC and IC measurements. A half-life of  $T_{1/2} = (270.99 \pm 0.19)$  d for  $^{68}\text{Ge}$  was obtained by measurements with an ionization chamber.

L17 ANSWER 45 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1982:467389 HCAPLUS  
 DOCUMENT NUMBER: 97:67389  
 TITLE: Immune complex type disease induced by mercury(II) chloride in Brown-Norway rats: genetic control of susceptibility  
 AUTHOR(S): Sapin, Catherine; Mandet, Chantal; Druet, Elvira;  
**Gunther, E.**; Druet, P.  
 CORPORATE SOURCE: Hop. Broussais, Paris, 75674/14, Fr.  
 SOURCE: Clinical and Experimental Immunology (1982), 48(3),  
 700-4  
 CODEN: CEXIAL; ISSN: 0009-9104  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB HgCl<sub>2</sub> induces a biphasic autoimmune glomerulonephritis in Brown-Norway (BN) rats, but not in Lewis (LEW) rats. The genetic control of susceptibility to both phases was investigated by testing the response of

segregants between BN and LEW rats and congenic LEW.1N rats. The susceptibility to the 1st phase, characterized by the appearance of antiglomerular basement membrane antibodies, depends on several genes 1 of which is RT1 linked. Susceptibility to the 2nd phase, which is an immune complex type glomerulonephritis, depended on 1 major RT1-linked gene or cluster of genes with a role for other(s) non-RT1 linked gene(s) controlling the magnitude of the response. However, congenic LEW.1N rats were resistant. Thus, the disease gene was lost during the strain derivation. The question of whether both phases are 2 different diseases or expression of the same process cannot be definitely answered; data however indicate a dissociation of disease processes.

L17 ANSWER 46 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1958:117472 HCAPLUS

DOCUMENT NUMBER: 52:117472

ORIGINAL REFERENCE NO.: 52:20822h-i

TITLE: The trace elements as integral constituents of ferments and their importance in agriculture

AUTHOR(S): Gunther, E.

SOURCE: Deut. Landwirtschaft (1956), 7, 332-7

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB The influence of B, Co, Ni, Zn, Cu, Mn, Al, Mo, and Fe on the health of plants is discussed. Ranges in p.p.m. of these elements contained in various plants and soils are given. 32 references.

L17 ANSWER 47 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1956:87249 HCAPLUS

DOCUMENT NUMBER: 50:87249

ORIGINAL REFERENCE NO.: 50:16405d-e

TITLE: Stereoisomerism and excited states of simple polymethine dyes

AUTHOR(S): Baumgartner, F.; Gunther, E.; Scheibe, G.

CORPORATE SOURCE: Tech. Hochschule, Munich, Germany

SOURCE: Zeitschrift fuer Elektrochemie und Angewandte

Physikalische Chemie (1956), 60, 570-2

CODEN: ZEAPAA; ISSN: 0372-8323

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB 1,5-N,N'-dipyrrolidylpentamethine perchlorate (I) is converted by irradiation with light of wave length 424 mμ (the principal absorption band of I) at -144° into a compound (II) with principal absorption band at 454 mμ. II reverts to I spontaneously at higher temps. with an activation energy of 5.7 kcal. I and II show fluorescence bands at 440 and 470 mμ, resp.

L17 ANSWER 48 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1952:46417 HCAPLUS

DOCUMENT NUMBER: 46:46417

ORIGINAL REFERENCE NO.: 46:7713e

TITLE: Vitamin C content of Germany's main medicinal and spice plants

AUTHOR(S): Gunther, E.; Heeger, E. F.; Rosenthal, Christine

SOURCE: Pharmazie (1952), 7, 24-50

CODEN: PHARAT; ISSN: 0031-7144

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB The vitamin C content of various samples of different parts of 81 varieties of plants was determined at different times.



L17 ANSWER 49 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1950:36771 HCAPLUS  
 DOCUMENT NUMBER: 44:36771  
 ORIGINAL REFERENCE NO.: 44:7026h-i,7027a  
 TITLE: Determination of the ascorbic acid oxidation power [oxidase] in plants and animal organs and tissues  
 AUTHOR(S): Gunther, E.  
 SOURCE: Pharmazie (1948), 3, 158-61  
 CODEN: PHARAT; ISSN: 0031-7144  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable

AB The ascorbic acid content and the oxidase activity have been measured under various conditions in different parts of a variety of plants. There is no relation between the 2 quantities. The oxidase activity is greatly retarded by frost, completely inhibited at -20°, and destroyed by heating to 100°. Oxidase activity increases and ascorbic acid content decreases as the plants wither. The results do not support Wachholder's exchange theory.

L17 ANSWER 50 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1948:42772 HCAPLUS  
 DOCUMENT NUMBER: 42:42772  
 ORIGINAL REFERENCE NO.: 42:8983h-i  
 TITLE: The supplying of the population with natural sources of vitamin C  
 AUTHOR(S): Schwarze, W. K.; Gunther, E.  
 CORPORATE SOURCE: Anst. Vitaminforschung u. Vitaminprufung, Leipzig, Germany  
 SOURCE: Pharmazie (1946), 1, 320-2  
 From: Chem. Zentr. I, 534-5(1947).  
 CODEN: PHARAT; ISSN: 0031-7144  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable

AB The vitamin C content of blackberry, raspberry, strawberry, birch, elderberry, walnut, violet, linden, poplar, dog-rose, and privet leaves, of linden blossoms, of mixts. of grasses, and of hip varies with the season. It is almost completely lost by simple drying or salting down of the fresh plant parts. Blanching of the coarsely cut fresh plants with steam (to destroy the enzymes) and subsequent drying in vacuum or in an ordinary drying oven at 60-90° is recommended.

L17 ANSWER 51 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1948:42771 HCAPLUS  
 DOCUMENT NUMBER: 42:42771  
 ORIGINAL REFERENCE NO.: 42:8983h-i  
 TITLE: The supplying of the population with natural sources of vitamin C  
 AUTHOR(S): Schwarze, W. K.; Gunther, E.  
 CORPORATE SOURCE: Anst. Vitaminforschung u. Vitaminprufung, Leipzig, Germany  
 SOURCE: Pharmazie (1946), 1, 320-2  
 CODEN: PHARAT; ISSN: 0031-7144  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable

AB The vitamin C content of blackberry, raspberry, strawberry, birch, elderberry, walnut, violet, linden, poplar, dog-rose, and privet leaves, of linden blossoms, of mixts. of grasses, and of hip varies with the season. It is almost completely lost by simple drying or salting down of the fresh plant parts. Blanching of the coarsely cut fresh plants with

steam (to destroy the enzymes) and subsequent drying in vacuum or in an ordinary drying oven at 60-90° is recommended.

L17 ANSWER 52 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1947:29416 HCAPLUS

DOCUMENT NUMBER: 41:29416

ORIGINAL REFERENCE NO.: 41:5915d-f

TITLE: The determination of L-ascorbic acid by chemical methods

AUTHOR(S): Schwarze, W. K.; Gunther, E.

CORPORATE SOURCE: Lab. for Vitamin Research and Vitamin Testing for the Soviet Zone of Occupation, Leipzig

SOURCE: Pharmazie (1946), 1, 153-7  
From: Chem. Zentr. 1947, I, 79.  
CODEN: PHARAT; ISSN: 0031-7144

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB It is shown that the wide variation of results in the determination of vitamin C

by titration with 2,6-dichlorophenolindophenol is due less to the method used than to the preliminary treatment of the sample and the preparation of the extract The reducing substances other than the ascorbic acid should be

determined

and this value taken into consideration in the calcn. Expts. reported show that in the determination of the "blank" the ascorbic acid is destroyed

by Cu

salts if some HCl is added to the metaphosphate solution Moreover, the combined ascorbic acid is hydrolyzed so that the total vitamin C is determined

L17 ANSWER 53 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1941:35801 HCAPLUS

DOCUMENT NUMBER: 35:35801

ORIGINAL REFERENCE NO.: 35:5605g

TITLE: Solution of ground water problems by means of flow in thin layers

AUTHOR(S): Gunther, E.

SOURCE: Wasser und Abwasser (Leipzig) (1940), 38, 66  
CODEN: WAABA9

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Elec. and sand models are used to determination the flow of ground water.

L17 ANSWER 54 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1941:35800 HCAPLUS

DOCUMENT NUMBER: 35:35800

ORIGINAL REFERENCE NO.: 35:5605g

TITLE: Solution of ground water problems by means of flow in thin layers

AUTHOR(S): Gunther, E.

SOURCE: Wasserkraft u. Wasserwirt. (1940) 49-55

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Elec. and sand models are used to determination the flow of ground water.

L17 ANSWER 55 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1937:61433 HCAPLUS

DOCUMENT NUMBER: 31:61433

ORIGINAL REFERENCE NO.: 31:8469f-g

TITLE: Rolling and sticking of sheet

AUTHOR(S): Gunther, E.

SOURCE: Stahl und Eisen (1937), 57, 601-4  
 CODEN: STEIA3; ISSN: 0340-4803  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB P, Si and to some extent C cause less sticking. High-Si transformer sheet, higher-C sheet, and alloy sheet stick so little that the rolling temperature and pressure must actually be increased to give some sticking so as to get proper rolling. Thinner sheet sticks more. Keeping the rolling pressure more uniform will make the sheet more easily separated

L17 ANSWER 56 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1934:1184 HCAPLUS  
 DOCUMENT NUMBER: 28:1184  
 ORIGINAL REFERENCE NO.: 28:184e-f  
 TITLE: Emulsin. XII. 1. The cleavage of phenol- $\beta$ -d-isorhamnoside by emulsin  
 AUTHOR(S): Helferich, B.; Rohr, H.; Gunther, E.  
 SOURCE: Z. physiol. Chem. (1933), 221, 90-2  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB cf. C. A. 27, 2959. Phenol- $\beta$ -d-isorhamnoside, m. 161-2°, [ $\alpha$ ]D<sub>21</sub> -80.8°, was obtained by hydrolysis of the tri-Ac derivative, m. 134-5°, [ $\alpha$ ]D<sub>21</sub> in CHCl<sub>3</sub> -7.3°, prepared by Zn reduction of triacetyl-phenol- $\beta$ -d-glucoside-6-bromohydrin. It is hydrolyzed by almond emulsin about twice as rapidly as the corresponding glucoside. The activity of this enzyme is strictly parallel for the 2 substrates, in different stages of enzyme purification and damage by heat or ultra-violet rays. There is no occasion to assume the existence of a specific isorhamnosidase.

L17 ANSWER 57 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1933:33542 HCAPLUS  
 DOCUMENT NUMBER: 27:33542  
 ORIGINAL REFERENCE NO.: 27:3021f-g  
 TITLE: Adaptation of the seedling method to the examination of moor soils  
 AUTHOR(S): Brune, F.; Arnd, T.; Gunther, E.; Poock, A.  
 SOURCE: Zeitschrift fuer Pflanzenernaehrung, Duengung, Bodenkunde (1932), 26A, 271-83  
 CODEN: ZPDBAQ; ISSN: 0372-9702  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB The use of fresh soil samples, measured by volume, is recommended. If necessary, CaCO<sub>3</sub> is added to give an equivalent of 4000 kg. of CaO per hectare. After the growth of the barley plants, roots are cut off immediately beneath the seed and analyses made of the upper portion only.

L17 ANSWER 58 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1932:39234 HCAPLUS  
 DOCUMENT NUMBER: 26:39234  
 ORIGINAL REFERENCE NO.: 26:4070c-g  
 TITLE: Emulsin. VII  
 AUTHOR(S): Helferich, B.; Winkler, S.; Gootz, R.; Peters, O.; Gunther, E.  
 SOURCE: Z. physiol. Chem. (1932), 208, 91-100  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB cf. C. A. 26, 3268. Emulsin solns. obtained by extracting the powdered press cake of sweet almonds with dilute ZnSO<sub>4</sub>, precipitating with tannin, extracting the precipitate with

Me<sub>2</sub>CO and dissolving the residue in H<sub>2</sub>O, may be purified tenfold by treatment with Ag<sub>2</sub>O. The solution is first treated with a small quantity of Ag<sub>2</sub>O, then filtered and the residue discarded. A larger quantity of Ag<sub>2</sub>O is added to the filtrate, and the resulting precipitate decomposed by H<sub>2</sub>S. The final filtrate contains the enzyme. Several repetitions of this process yield a product with greatly increased activity per unit weight of dry substance. Six phenol glucosides were used as substrates, viz., the  $\beta$ -d-galactoside (I),  $\alpha$ -d-galactoside (II),  $\alpha$ -l-arabinoside (III),  $\beta$ -l-arabinoside (IV),  $\beta$ -d-xyloside (V) and  $\beta$ -d-glucoside-6-bromohydrin (VI). The Ag<sub>2</sub>O treatment greatly increased the enzymic activity toward I, III, V, VI and salicin, but greatly diminished the activity toward II and IV. Similarities in the configuration of I, III, V and VI are pointed out which support the assumption that all are hydrolyzed by one and the same enzyme. The following alterations in the structure of a  $\beta$ -glucoside do not interfere with the activity of  $\beta$ -glucosidase: The 6-hydroxyl may be replaced by Br (VI), the terminal CH<sub>2</sub>OH may be replaced by H (V), the configuration at the 4-C may be reversed from d to l (I), and here again the terminal CH<sub>2</sub>OH replaced by H (III). The enzyme is therefore not sensitive to alterations in the substrate at the 4- or the 6-C atom. All 4 substrates have the same configuration at the 1-C. If this configuration is altered (II and IV), the cleavage by the purified enzyme is so small as to represent quite a different order of magnitude. A new derivative described is phenol- $\alpha$ -l-arabinoside (III), m. 153-5°,  $[\alpha]_{D17}^{20} 6.0^\circ$ , obtained by NaOMe hydrolysis of the triacetate, m. 87-9°,  $[\alpha]_{D19}^{20} 24.7^\circ$ , which in turn was prepared by condensation of PhOH in quinoline with acetobromoarabinose and Ag<sub>2</sub>O.

L17 ANSWER 59 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1932:12351 HCAPLUS

DOCUMENT NUMBER: 26:12351

ORIGINAL REFERENCE NO.: 26:1359h-i

TITLE: Can the freshness of forages be determined from their free fatty acid content?

AUTHOR(S): Gunther, E.

SOURCE: Chimie et Industrie (Paris) (1931), 26, 1187

CODEN: CHIEAN; ISSN: 0009-4358

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB The estimation of the freshness of forage or feeds by determination of the free fatty

acids gives satisfactory results with the press cakes of oil-bearing plants, but is not suitable for meat and fish meals and brans.

Considerable data are given on the permissible limits of free fatty acids, fat contents, degree of rancidity and development of molds in a number of vegetable press cakes. In animal products, addition of NaCl retards the decomposition of the glycerides and prevents mold formation. Another important indication regarding the state of preservation of feeds is the presence of living mites, which require a certain amount of moisture to live.

L17 ANSWER 60 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1932:12350 HCAPLUS

DOCUMENT NUMBER: 26:12350

ORIGINAL REFERENCE NO.: 26:1359h-i

TITLE: Can the freshness of forages be determined from their free fatty acid content?

AUTHOR(S): Gunther, E.

SOURCE: Fortschritte der Landwirtschaft (1931), 6, 243-6

CODEN: FLWSAQ; ISSN: 0367-2557

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB The estimation of the freshness of forage or feeds by determination of the free fatty acids gives satisfactory results with the press cakes of oil-bearing plants, but is not suitable for meat and fish meals and brans. Considerable data are given on the permissible limits of free fatty acids, fat contents, degree of rancidity and development of molds in a number of vegetable press cakes. In animal products, addition of NaCl retards the decomposition of the glycerides and prevents mold formation. Another important indication regarding the state of preservation of feeds is the presence of living mites, which require a certain amount of moisture to live.

L17 ANSWER 61 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1932:6694 HCAPLUS

DOCUMENT NUMBER: 26:6694

ORIGINAL REFERENCE NO.: 26:792e-f

TITLE: Action of frost on various arable soils and the resulting effect on the growth of oats and barley

AUTHOR(S): Gunther, E.

SOURCE: Landwirtschaftliche Jahrbuecher (1931), 73, 893-922  
CODEN: LWSJAK; ISSN: 0368-8194

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB G. describes apparatus developed to study the effect of freezing. Pore space, hygroscopicity and water capacity are studied. Freezing affects all these in acid soil but has no effect on soil containing chalk. The water content is an important factor in frost action. Freezing had no effect on adsorption of soils. Freezing improved the intake of K and P of these plants which G. assumes is due to improvement in phys. condition.

L17 ANSWER 62 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1931:12330 HCAPLUS

DOCUMENT NUMBER: 25:12330

ORIGINAL REFERENCE NO.: 25:1350c

TITLE: Waste-gas utilization from the muffle furnace

AUTHOR(S): Gunther, E.

SOURCE: Sprechsaal (1930), 63, 975  
CODEN: SPREAS; ISSN: 0341-0676

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Unavailable

L17 ANSWER 63 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1928:20739 HCAPLUS

DOCUMENT NUMBER: 22:20739

ORIGINAL REFERENCE NO.: 22:2431g-h

TITLE: The examination of the Mitscherlich procedure for the determination of the fertilizer requirements of soils

AUTHOR(S): Gerlach, M.; Gunther, E.; Seidel, C.

SOURCE: Zeitschrift fuer Pflanzenernaehrung, Duengung, Bodenkunde (1928), 11A, 1-29  
CODEN: ZPDBAQ; ISSN: 0372-9702

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C. A. 22, 1008. The expts. carried out by the authors show that Mitscherlich cannot satisfactorily use the value of the growth factor constant and consequently the law founded on it. In the Mitscherlich equation, the total quantities of the nutrient materials used in the test must not be used, but only the part of the nutrients absorbed by the plant. The value of the growth factor constant is not constant The percent

increase in yield in two expts. is only equal when, besides the material tested, other growth factors such as the basic fertilization and the water are applied in the same amts. Therefore, the use of the Mitscherlich yield tables is not generally applicable. The Mitscherlich procedure for the determination of the fertilizer requirements of the soil gives no more than a well-conducted vegetation experiment would give.

L17 ANSWER 64 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1928:13971 HCAPLUS  
 DOCUMENT NUMBER: 22:13971  
 ORIGINAL REFERENCE NO.: 22:1644h-i  
 TITLE: Investigations on the Neubauer seedling method  
 AUTHOR(S): Gunther, E.  
 SOURCE: Zeitschrift fuer Pflanzenernaehrung, Duengung, Bodenkunde (1927), 6B, 502-6  
 CODEN: ZPDBAQ; ISSN: 0372-9702  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable

AB cf. C. A. 21, 2348. Even with uniform seed, errors are associated with the method. After harvest of the seedlings, soil-sand mixture must be elutriated to determine the total mass of roots; and this introduces sources of error. Expts. showed that seedlings far from assimilated all the root-soluble nutrients in the soil.

L17 ANSWER 65 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1927:19043 HCAPLUS  
 DOCUMENT NUMBER: 21:19043  
 ORIGINAL REFERENCE NO.: 21:2348a-b  
 TITLE: Neubauer's "seedling" method for determining fertilizer requirements of soils  
 AUTHOR(S): Gunther, E.  
 SOURCE: Z. Pflanzenernahr. Dungung (1926), B5, 32-6  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable

AB Critical expts. on Neubauer's method for determining the P2O5 and K requirements of soils show that considerable variations in the light intensity during growth of the seedlings affect the percentage of nutrients absorbed to a small extent only. Similarly, the absorption of nutrients by the seedlings is almost unaffected by changing the pH of a soil from an initial value of 5.0 to 6.5 and 8.0 by addition of CaCO3. Under normal conditions, both light intensity and soil reaction can be neglected in carrying out the test.

L17 ANSWER 66 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1924:17949 HCAPLUS  
 DOCUMENT NUMBER: 18:17949  
 ORIGINAL REFERENCE NO.: 18:2402h-i  
 TITLE: The lime-phosphoric acid factor in relation to the Aereboe-Wrangell system of fertilizing  
 AUTHOR(S): Gunther, E.  
 SOURCE: Z. Pflanzenernahr. Dungung (1924), 3B, 17-26  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable

AB Crops were treated with various fertilizers designed to produce neutral, acid and alkaline conditions in the soil but containing equivalent plant food. From the ratio CaO:P2O5 computed from analyses of the plant ash no division into classes appeared possible as proposed by Wrangell. Variations in the

amount and proportion of CaO and P2O5 occurred in different plants on the same soil and in the same species on different soils. Plants take up relatively more CaO than P2O5 under acid conditions than they do under basic ones.

L17 ANSWER 67 OF 67 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1913:9055 HCAPLUS

DOCUMENT NUMBER: 7:9055

ORIGINAL REFERENCE NO.: 7:1329c

TITLE: The Hoepfner Zinc Chloride Electrolytic Process

AUTHOR(S): Gunther, E.

SOURCE: Metall und Erz (1913), 1, 206-7

CODEN: MERZAG; ISSN: 0368-9514

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB G. describes briefly the development of the process under Eschellmann who succeeded in producing electrolytic Zn 99-97% pure.

=> => d stat que nos l18

L5 STR

L7 118852 SEA FILE=REGISTRY SSS FUL L5

L8 STR

L9 157 SEA FILE=REGISTRY SUB=L7 SSS FUL L8

L10 STR

L11 18 SEA FILE=REGISTRY SUB=L9 SSS FUL L10

L12 7 SEA FILE=HCAPLUS ABB=ON PLU=ON L11

L15 43 SEA FILE=HCAPLUS ABB=ON PLU=ON ("EMIG P"/AU OR "EMIG PETER"/AU)

L16 41 SEA FILE=HCAPLUS ABB=ON PLU=ON L15 NOT L12

L17 67 SEA FILE=HCAPLUS ABB=ON PLU=ON ("GUNTHER E"/AU OR "GUNTHER ECKHARD"/AU) NOT (L12 OR L16)

L18 1 SEA FILE=HCAPLUS ABB=ON PLU=ON (("AUE B J"/AU OR "AUE BEATE"/AU)) NOT (L12 OR L16 OR L17)

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=> d ibib abs l18 1

L18 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1967:408125 HCAPLUS

DOCUMENT NUMBER: 67:8125

TITLE: Fumarate reductase activity of Streptococcus faecalis

AUTHOR(S): Aue, B. J.; Deibel, Robert H.

CORPORATE SOURCE: Cornell Univ., Ithaca, NY, USA

SOURCE: Journal of Bacteriology (1967), 93(6), 1770-6

CODEN: JOBAAAY; ISSN: 0021-9193

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Some characteristics of a fumarate reductase from *S. faecalis* are described. The enzyme had a pH optimum of 7.4; optimal activity was observed when the ionic strength of the phosphate buffer was adjusted to 0.088. The Km value of the enzyme for reduced flavine mononucleotide was  $2 + 10^{-4}M$  as determined with a 26-fold preparation. In addition to fumarate, the enzyme reduced maleate and mesaconate. No succinate dehydrogenase activity was detected, but succinate did act as an inhibitor of the fumarate reductase activity. Other inhibitors were malonate, citraconate,

and trans-,trans-muconate. Metal-chelating agents did not inhibit the enzyme. A limited inhibition by SH-binding agents was observed, and the preps. were sensitive to air oxidation and storage. Glycine, alanine, histidine, and possibly lysine stimulated fumarate reductase activity in the cell-free exts. However, growth in media supplemented with glycine did not enhance fumarate reductase activity. The enzymic activity appears to be constitutive. 16 references.

=> => d stat que l19 nos

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L5          STR
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L8          STR
L9          157 SEA FILE=REGISTRY SUB=L7 SSS FUL L8
L10         STR
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L16         41 SEA FILE=HCAPLUS ABB=ON PLU=ON L15 NOT L12
L17         67 SEA FILE=HCAPLUS ABB=ON PLU=ON ("GUNTHER E"/AU OR "GUNTHER
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L18         1 SEA FILE=HCAPLUS ABB=ON PLU=ON (("AUE B J"/AU OR "AUE
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=> d ibib abs l19 1-41

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L19 ANSWER 1 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:53914 HCAPLUS
DOCUMENT NUMBER: 144:150233
TITLE: Preparation of 1,2,3,4-tetrahydrocarbazoles as
          gonadotropin-releasing hormone receptor (LHRH)
          antagonist
INVENTOR(S): Paulini, Klaus; Gerlach, Matthias; Guenther, Eckhard;
          Polymeropoulos, Emmanuel; Baasner, Silke;
          Schmidt, Peter; Kuehne, Ronald; Soederhaell, Arvid
PATENT ASSIGNEE(S): Zentaris G.m.b.H., Germany; Solvay Pharmaceuticals
          B.V.
SOURCE: PCT Int. Appl., 113 pp.
          CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

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PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006005484	A1	20060119	WO 2005-EP7255	20050705
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				



RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,  
 IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,  
 CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,  
 GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,  
 KG, KZ, MD, RU, TJ, TM

DE 102004033902 A1 20060216 DE 2004-102004033902 20040714  
 US 2006014818 A1 20060119 US 2005-172142 20050630

PRIORITY APPLN. INFO.:

DE 2004-102004033902A 20040714  
 US 2004-587969P P 20040714  
 US 2005-683178P P 20050520

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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [X1 = S, O; X2, X3 = O with provisos; R1, R2 = H, aryl, alkyl, etc.; R3 = alkyl, arylalkyl, heteroarylalkyl, etc.; R4, R5, R6, R7 = H, halo, CN, etc.; R9 = H, alkyl, aryl, etc.; R10 = R11, COR11, CO2R11, etc.; R11 = alkyl, aryl, heteroaryl, etc.; R8 = alkylaryl, alkylheteroaryl, etc.; ] and their pharmaceutically acceptable salts were prepared For example, tetrahydrocarbazole II was prepared via solid phase synthesis from FmocValOH in 14% yield. In LHRH receptor binding assays, 7-examples of compds. I exhibited EC50 values ranging from 80-1.0 x 10<sup>-10</sup> M.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:544300 HCAPLUS

DOCUMENT NUMBER: 143:146816

TITLE: Antagonist and agonist binding models of the human gonadotropin-releasing hormone receptor

AUTHOR(S): Soederhaell, J. Arvid; Polymeropoulos, Emmanuel E.; Paulini, Klaus; Guenther, Eckhard; Kuehne, Ronald

CORPORATE SOURCE: Institute for Molecular Pharmacology, Berlin, D-13125, Germany

SOURCE: Biochemical and Biophysical Research Communications (2005), 333(2), 568-582

CODEN: BBRC A9; ISSN: 0006-291X

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB G-protein-coupled receptors (GPCRs) constitute one of the most important classes of drug targets. Since the first high-resolution structure of a GPCR was determined by K. Palczewski and co-workers (2000), development of in silico models of rhodopsin-like GPCRs could be rationally founded. In this work, we present a model of the human gonadotropin-releasing hormone receptor based on the rhodopsin structure. The transmembrane helices are modeled by homol., while the extra- and intracellular loops are modeled in such a way that exptl. determined interactions and microdomains (e.g., hydrophobic cores) are retained. We conclude that specifically tailored models, compared to more automatic approaches, have the benefit that known interactions are easily introduced early in the homol. modeling. Furthermore, tailored models, although more tedious to construct, are better suited for drug lead finding and for compound optimization. To test the stability of the receptor, we performed a 1 ns mol. dynamics simulation. Moreover, we docked two agonists (native GnRH and

Triptorelin) and two antagonists (Cetrorelix and the covalently constrained dicyclic decapeptide dicyclo(1,1'-5/4-10) [Ac-Glu1(Gly1')-DCpa2-DTrp3-Asp4-Dbu5-DNal6-Leu7-Arg8-Pro9-Dpr10-NH2]) into the putative receptor binding site. The docked ligand conformations result in ligand-receptor interactions that are generally in good agreement with site-directed mutagenesis and ligand-binding studies presented in the literature. Our results indicate that the binding conformation of the antagonists differs from that of the agonists. This difference can be linked to the activation or inhibition of the receptor.

REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 3 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:658086 HCAPLUS

DOCUMENT NUMBER: 137:185497

TITLE: Preparation of quinolines, isoquinolines and phthalazines as GnRH antagonists

INVENTOR(S): Strehlke, Peter; Droesch, Peter; Buehmann, Ulrich; Schmees, Norbert; Muhn, Peter; Hess-Stumpp, Holger; Kuehne, Roland; Guenther, Eckhard; **Polymeropoulos, Emmanuel**; Ter Laak, Antonius Marinus

PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 45 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

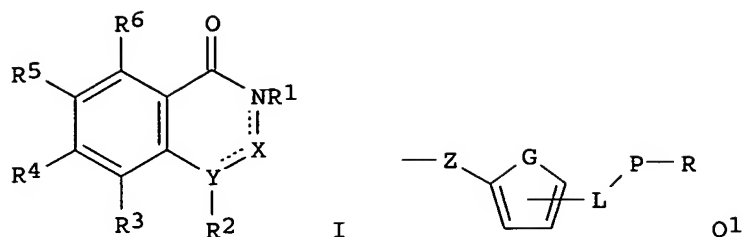
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002066437	A1	20020829	WO 2002-EP1882	20020221
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CA 2438709	AA	20020829	CA 2002-2438709	20020221
EP 1362034	A1	20031119	EP 2002-716803	20020221
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
BR 2002007451	A	20040601	BR 2002-7451	20020221
JP 2004528298	T2	20040916	JP 2002-565954	20020221
NZ 527597	A	20041029	NZ 2002-527597	20020221
NO 2003003698	A	20031020	NO 2003-3698	20030820
BG 108165	A	20040831	BG 2003-108165	20030909
PRIORITY APPLN. INFO.:			DE 2001-10108271	A 20010221
			US 2001-274914P	P 20010313
			WO 2002-EP1882	W 20020221

OTHER SOURCE(S): MARPAT 137:185497

GI



AB Title compds. [I; R1 = COR11, cyano, CO2R12, CONR12R13, etc.; R11, R12 = (saturated) (hetero)cyclyl, alkyl, (substituted) Ph, furanyl, thiophenyl; R13 = H, alkyl; R2 = CHR21R22, etc.; R21 = H, alkyl, (substituted) Ph; R22 = (substituted) Ph, naphthyl; R3 = H, alkyl; R4 = H, alkyl, halo; R5 = Q1; G = CH:CH, CH:N, N:CH, O, S; Z = bond, O, S, etc.; L = CH2, NH; P = CO, SOx; x = 0-2; R = (substituted) amino, (branched) (substituted) alkyl, 3-7 membered cycloalkyl; R6 = CH2NR61R62; R61 = H, alkyl; R62 = alkyl, (substituted) aralkyl], were prepared Thus, a mixture of N-benzylamine and N,N-diisopropylethylamine was added to 78 mg 6-(4-acetamidophenoxy)-5-(chloromethyl)-1-(2,6-difluorobenzyl)-1,4-dihydro-4-oxo-quinoline-3-carboxylic acid Et ester (preparation given) in DMF at 0° followed by stirring for 20 h at room temperature to give 70 mg 6-(4-acetamidophenoxy)-5-(N-benzyl-N-methylaminomethyl)-1-(2,6-difluorobenzyl)-1,4-dihydro-4-oxoquinoline-3-carboxylic acid Et ester. The anal. of the antagonistic activity is given.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:632477 HCAPLUS

DOCUMENT NUMBER: 137:154937

TITLE: Preparation of quinolines, isoquinolines and phthalazines as GnRH antagonists

INVENTOR(S): Strehlke, Peter; Driescher, Peter; Buehmann, Ulrich; Schmees, Norbert; Muhn, Peter; Hess-Stumpp, Holger; Kuehne, Roland; Guenther, Eckhard; Polymeropoulos, Emmanuel; Ter Laak, Antonius Marinus

PATENT ASSIGNEE(S): Schering A.-G., Germany

SOURCE: Ger. Offen., 18 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

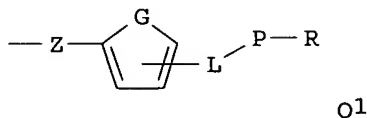
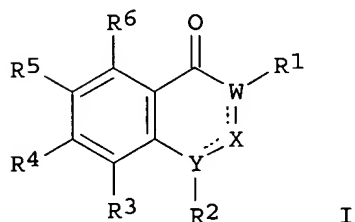
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10108271	A1	20020822	DE 2001-10108271	20010221
CA 2438709	AA	20020829	CA 2002-2438709	20020221
WO 2002066437	A1	20020829	WO 2002-EP1882	20020221

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,

UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,  
 CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,  
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2003105328	A1	20030605	US 2002-78530	20020221
US 6790858	B2	20040914		
EP 1362034	A1	20031119	EP 2002-716803	20020221
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
CN 1496354	A	20040512	CN 2002-806359	20020221
BR 2002007451	A	20040601	BR 2002-7451	20020221
JP 2004528298	T2	20040916	JP 2002-565954	20020221
NZ 527597	A	20041029	NZ 2002-527597	20020221
ZA 2003006429	A	20040211	ZA 2003-6429	20030819
NO 2003003698	A	20031020	NO 2003-3698	20030820
BG 108165	A	20040831	BG 2003-108165	20030909
US 2005004127	A1	20050106	US 2004-896961	20040723
PRIORITY APPLN. INFO.:				
			DE 2001-10108271	A 20010221
			US 2001-274914P	P 20010313
			US 2002-78530	A3 20020221
			WO 2002-EP1882	W 20020221

OTHER SOURCE(S): MARPAT 137:154937  
 GI

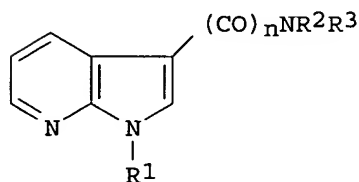


AB Title compds. [I; R1 = COR11, cyano, CO2R12, CONR12R13, etc.; R11, R12 = (saturated) cyclyl, heterocyclyl, alkyl, (substituted) Ph, furanyl, thiophenyl; R13 = H, alkyl; R2 = CHR21R22, etc.; R21 = H, alkyl, (substituted) Ph; R22 = (substituted) Ph, naphthyl; R4 = H, alkyl, halo; R5 = Q1; G = C:C, C:N, N:C, O, S; Z = bond, O, S, etc.; L = CH2, NH; P = CO, SOx; x = 0-2; R = (substituted) amino, (branched) alkyl, 3-7 membered cycloalkyl; R6 = CH2NR61R62; R61 = H, alkyl; R62 = alkyl, (substituted) aralkyl, heteroarylalkyl, etc.], were prepared Thus, N-benzylamine and N,N-diisopropylethylamine was added to 78 mg 6-(4-acetamidophenoxy)-5-(chloromethyl)-1-(2,6-difluorobenzyl)-1,4-dihydro-4-oxoquinoline-3-carboxylic acid Et ester (preparation given) in DMF at 0° followed by stirring for 20 h at room temperature to give 70 mg 6-(4-acetamidophenoxy)-5-(N-benzyl-N-methylaminomethyl)-1-(2,6-difluorobenzyl)-1,4-dihydro-4-oxoquinoline-3-carboxylic acid Et ester. The anal. of the antagonistic activity is given.

L19 ANSWER 5 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2002:332190 HCAPLUS  
 DOCUMENT NUMBER: 136:340669  
 TITLE: Novel 7-azaindolecarboxamides as phosphodiesterase 4 inhibitors  
 INVENTOR(S): Hoefgen, Norbert; Egerland, Ute; Kronbach, Thomas;

Marx, Degenhard; Szelenyi, Stefan; Kuss, Hildegard;  
**Polymeropoulos, Emmanuel**  
 PATENT ASSIGNEE(S): Arzneimittelwerk Dresden GmbH, Germany  
 SOURCE: PCT Int. Appl., 55 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002034747	A1	20020502	WO 2001-EP12376	20011025
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10053275	A1	20020502	DE 2000-10053275	20001027
CA 2428468	AA	20020502	CA 2001-2428468	20011025
AU 2002021753	A5	20020506	AU 2002-21753	20011025
EP 1330455	A1	20030730	EP 2001-988718	20011025
EP 1330455	B1	20050803		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
EE 200300166	A	20030815	EE 2003-166	20011025
BR 2001014903	A	20031014	BR 2001-14903	20011025
JP 2004512337	T2	20040422	JP 2002-537738	20011025
NZ 525369	A	20040924	NZ 2001-525369	20011025
AT 301121	E	20050815	AT 2001-988718	20011025
RU 2268887	C2	20060127	RU 2003-115621	20011025
NO 2003001722	A	20030414	NO 2003-1722	20030414
BG 107725	A	20040831	BG 2003-107725	20030416
ZA 2003003236	A	20030731	ZA 2003-3236	20030425
HR 2003000427	A1	20030831	HR 2003-427	20030526
US 2004106641	A1	20040603	US 2003-399051	20030617
HK 1053839	A1	20051028	HK 2003-106201	20030829
PRIORITY APPLN. INFO.:			DE 2000-10053275	A 20001027
			US 2000-244342P	P 20001030
			WO 2001-EP12376	W 20011025
OTHER SOURCE(S):			CASREACT 136:340669; MARPAT 136:340669	
GI				



AB 7-Azaindoles I [n = 1, 2; R1 = (un)substituted alkyl, alkenyl; R2, R3 = H, (un)substituted alkyl, Ph, pyridyl, uracilyl, triazolyl; NR2R3 =

morpholino, thiomorpholino, thiomorpholine S,S-dioxide, 4-methylpiperazino] were prepared for use as PDE-4 inhibitors. Thus, 1-cyclopropylmethyl-7-azaindole-3-carboxylic acid was converted to the acid chloride and treated with 4-aminomethylpyridine to give the amide which had an IC<sub>50</sub> for PDE-4 inhibition of 0.710  $\mu$ mol./L.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 6 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:883023 HCAPLUS

DOCUMENT NUMBER: 134:360953

TITLE: A peptidic binding site model for PDE 4 inhibitors

AUTHOR(S): Polymeropoulos, E. E.; Hofgen, N.

CORPORATE SOURCE: Corporate R&D, ASTA Medica Group, Department of

Chemical Research, Frankfurt, D-60314, Germany  
SOURCE: Molecular Modeling and Prediction of Bioactivity, [Proceedings of the European Symposium on Quantitative Structure-Activity Relationships: Molecular Modeling and Prediction of Bioactivity], 12th, Copenhagen, Denmark, Aug. 23-28, 1998 (2000), Meeting Date 1998, 395-396. Editor(s): Gundertofte, Klaus; Jorgensen, Flemming Steen. Kluwer Academic/Plenum Publishers: New York, N. Y.

CODEN: 69ASO3

DOCUMENT TYPE: Conference

LANGUAGE: English

AB Selective inhibitors of the isoenzyme phosphodiesterase 4 (PDE 4) have attracted increased interest as potential drugs for the treatment of allergic diseases such as asthma. The pharmacophore requirements for inhibiting catalytic activity have been recently analyzed. To further refine this pharmacophore model and define a peptidic model for PDE 4 inhibitors that has the ability to semi-qual. predict inhibitory activity, the program PrGen has been used.

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 7 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:567784 HCAPLUS

DOCUMENT NUMBER: 133:272153

TITLE: Langmuir Monolayers with Fluorinated Groups in the Hydrophilic Head. 1. Comparison of Trifluoroethyl Behenate and Ethyl Behenate Monolayers: Molecular Models, Mechanical Properties, Stability

AUTHOR(S): Petrov, J. G.; Polymeropoulos, E. E.;

Moehwald, H.

CORPORATE SOURCE: Max-Planck Institute of Colloids and Interfaces, Golm/Potsdam, D-14476, Germany

SOURCE: Langmuir (2000), 16(19), 7411-7420

CODEN: LANGD5; ISSN: 0743-7463

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In a series of three related papers we compare mech. properties and stability, morphol. and structure, and electrostatic potential and ellipsometric thickness of trifluoroethyl behenate (TFEB) and Et behenate (EB) Langmuir monolayers. The aim of these papers is to study the effect of fluorination of a Me group in the hydrophilic head on monolayer properties and structure. In the present Part 1 we show that trifluoroethyl ester forms significantly more unstable films with higher compressibility (lower compressional modulus) than the unsubstituted Et

ester. Both TFEB and EB surface pressure-area isotherms show compression-expansion hysteresis, but this hysteresis is larger for the fluorinated ester. The surface pressure-area loop of TFEB is shifted to larger mol. areas as compared to EB and gives larger limiting mol. areas at zero compression. This points to different vols. and/or conformations of the fluorinated and nonsubstituted hydrophilic heads. Maps of mol. lipophilicity and mol. electrostatic potential, based on semiempirical quantum mech. models of the two mols. in vacuo, relate the observed differences in monolayer properties to decreased hydrophilicity of the trifluoroethyl group and a stronger electrostatic repulsion between the hydrocarbon chains of TFEB. Such a repulsion results from polarization of the CH<sub>2</sub> groups adjacent to the heads that is more significant for the trifluoroethyl behenate mol.

REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 8 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:55462 HCAPLUS

DOCUMENT NUMBER: 132:202635

TITLE: A peptidic binding site model for PDE 4 inhibitors

AUTHOR(S): Polymeropoulos, Emmanuel E.; Hofgen, Norbert

CORPORATE SOURCE: Department of Chemical Research, Corporate R and D  
ASTA Medica Group, Frankfurt, D-60314, Germany

SOURCE: Quantitative Structure-Activity Relationships (1999),  
18(6), 543-547

CODEN: QSARDI; ISSN: 0931-8771

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The pseudoreceptor modeling program PrGen was used to construct a peptidic binding site model for phosphodiesterase 4 inhibitors. A training set of 21 diverse compds. (rolipram, nitraquazone and xanthine derivs., imidazo pyrido pyrazinones and 5-oxyindoles) was used to construct the binding site surrogate consisting of five amino acid residues, a Zn<sup>2+</sup> cofactor and an envelope of charged virtual particles. The model was validated by predicting the free energies of binding  $\Delta G_{pred0}$  of ten ligands (rolipram, imidazo pyrido pyrazinones and 5-oxyindoles). In seven cases the prediction was satisfactory. The rms deviation [4] in  $\Delta G_0$  is 0.16 and 1.82 kcal/mol-resulting in an uncertainty in IC<sub>50</sub> (or K<sub>i</sub>) of 1.32 and 22.81-for the training and the test set resp., while the corresponding maximal prediction errors in  $\Delta G_{pred0}$  were 0.27 kcal/mol and 4.50 kcal/mol.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 9 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:708761 HCAPLUS

DOCUMENT NUMBER: 131:310549

TITLE: New hydroxyindoles and their use as phosphodiesterase  
4 and TNF $\alpha$  inhibitors

INVENTOR(S): Hofgen, Norbert; Egerland, Ute; Poppe, Hildegard;  
Marx, Degenhard; Szelenyi, Stefan; Kronbach, Thomas;  
Polymeropoulos, Emmanuel; Heer, Sabine

PATENT ASSIGNEE(S): Arzneimittelwerk Dresden GmbH, Germany

SOURCE: PCT Int. Appl., 45 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

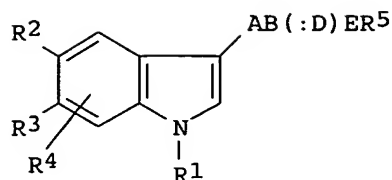
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9955696	A1	19991104	WO 1999-EP2792	19990424
W: AU, BG, BR, BY, CN, CZ, EE, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LT, LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, UZ, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
DE 19818964	A1	19991104	DE 1998-19818964	19980428
DE 19917504	A1	20001019	DE 1999-19917504	19990417
AU 9938229	A1	19991116	AU 1999-38229	19990424
AU 748403	B2	20020606		
BR 9910029	A	20001226	BR 1999-10029	19990424
TR 200003130	T2	20010122	TR 2000-200003130	19990424
EP 1076657	A1	20010221	EP 1999-920779	19990424
EP 1076657	B1	20040804		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002513017	T2	20020508	JP 2000-545856	19990424
NZ 507406	A	20021126	NZ 1999-507406	19990424
RU 2217422	C2	20031127	RU 2000-129678	19990424
AT 272631	E	20040815	AT 1999-920779	19990424
EP 1475377	A1	20041110	EP 2004-18391	19990424
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY				
PT 1076657	T	20041130	PT 1999-920779	19990424
ES 2222706	T3	20050201	ES 1999-920779	19990424
CA 2270301	AA	19991028	CA 1999-2270301	19990428
US 6251923	B1	20010626	US 1999-300973	19990428
TW 530048	B	20030501	TW 1999-88106886	19990428
ZA 2000005540	A	20010327	ZA 2000-5540	20001010
BG 104842	A	20011031	BG 2000-104842	20001011
NO 2000005454	A	20001207	NO 2000-5454	20001027
HK 1035183	A1	20050415	HK 2001-105669	20010814
US 2002111351	A1	20020815	US 2002-80821	20020221
US 6545025	B2	20030408		
US 2002115651	A1	20020822	US 2002-81395	20020221
US 6545158	B2	20030408		
US 2002119971	A1	20020829	US 2002-81642	20020221
US 2002137745	A1	20020926	US 2002-81807	20020221
US 6602890	B2	20030805		
US 38624	E	20041012	US 2002-176435	20020919
US 2003134876	A1	20030717	US 2003-347659	20030120
US 6613794	B2	20030902		
US 2004220183	A1	20041104	US 2004-856034	20040527
PRIORITY APPLN. INFO.:			DE 1998-19818964	A 19980428
			DE 1999-19917504	A 19990417
			EP 1999-920779	A3 19990424
			WO 1999-EP2792	W 19990424
			US 1999-300973	A3 19990428
			US 2000-653685	A3 20000901
			US 2002-81642	A1 20020221
			US 2002-81807	A3 20020221
OTHER SOURCE(S) :			MARPAT 131:310549	
GI				





AB Hydroxyindoles I [R1, R5 = (un)substituted aliphatic, carbocyclic, heterocyclic, spirocyclic; R2, R3 = H, OH,  $\geq 1$  of them being OH; R4 = H, (un)substituted OH, SH, S(O)H, SO<sub>2</sub>H, CO<sub>2</sub>H, C(S)OH, NO<sub>2</sub>, CN, F, Cl, Br, I; A = alkylene, alkenylene, (CHOZ)<sub>m</sub>, CO, CS, C:NZ, O, S, NZ; Z = (un)substituted alkyl, alkenyl, carbocyclic, heterocyclic; B = C, S, SO; D = O, S, CH<sub>2</sub>, NZ; E = bond, (CH<sub>2</sub>)<sub>m</sub>, O, S, NZ; m = 0-3] were prepared I have IC<sub>50</sub> for PDE IV inhibition of 1X10<sup>-9</sup>-1X10<sup>-5</sup> and a selectivity relative to PDE's 2, 3, and 5 of 100-10,000. N-(3,5-dichloro-4-pyridyl)-2-[1-(4-fluorobenzyl)-5-methoxy-3-indolyl]-2-oxoacetamide was obtained by demethylation of the 5-methoxy compound and was reduced to the 2-hydroxyacetamide with NaBH<sub>4</sub>.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 10 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:469510 HCAPLUS

DOCUMENT NUMBER: 129:169977

TITLE: The real gordian knot. Racemic mixtures versus pure enantiomers

AUTHOR(S): Szelenyi, I.; Geisslinger, G.; Polymeropoulos, E.; Paul, W.; Herbst, M.; Brune, K.

CORPORATE SOURCE: Arzneimittelwerk Dresden, Radebeul, D-01445, Germany

SOURCE: Drug News & Perspectives (1998), 11(3), 139-160  
CODEN: DNPEED; ISSN: 0214-0934

PUBLISHER: Prous Science

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review with 225 refs. is given on racemic mixts. and enantiomers of drugs. There are often pharmacodynamic, pharmacokinetic, and/or toxicol. differences between enantiomers. The choice between developing a racemate or single enantiomers depends on therapeutic advances and developmental costs involved. Regarding the target environment for drug intervention, even if natural physiol. mediators are achiral, their receptors may demonstrate a preference for the (-)- or (+)-enantiomer of agonists or antagonists. It is also obvious that the majority of enzymes and channels are stereospecific, at least to a variable extent. From a pharmacokinetics point of view, chirality can have an influence on drug absorption, distribution, metabolism, and elimination. With a few exceptions, toxicol. differences between isomers of known drugs are less dramatic than thought to be and only seldom substantiate the necessity of a racemic switch. The pharmaceutical industry is currently very interested in the so-called "racemic switch.". Before proceeding to a racemic switch it is necessary to determine if (1) it is chemical feasible to produce a single enantiomer, (2) a clin. advantage is obtainable through a racemic switch, and (3) a marketing advantage is obtainable. The real goal of a racemic switch should be the rational development of compds. that are profitable for the company and beneficial for the patient.

REFERENCE COUNT: 225 THERE ARE 225 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

## FORMAT

L19 ANSWER 11 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:744797 HCAPLUS

DOCUMENT NUMBER: 128:30427

TITLE: Chemistry and molecular biology in the search for new LHRH antagonists

AUTHOR(S): Kutscher, Bernhard; Bernd, Michael; Beckers, Thomas; Polymeropoulos, Emmanuel E.; Engel, Jurgen

CORPORATE SOURCE: ASTA Med. AG, Konzernforsch., Frankfurt, D-60315, Germany

SOURCE: Angewandte Chemie, International Edition in English (1997), 36(20), 2149-2161

CODEN: ACIEAY; ISSN: 0570-0833

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review, with 137 refs., discussing LHRH peptides as therapeutic agonists and antagonists of tumor growth, their structure and conformation, LHRH receptor assays, comparison of clin. relevant antagonists, LHRH receptor modeling, and the search for peptidomimetics for the LHRH receptor.

REFERENCE COUNT: 156 THERE ARE 156 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 12 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:549055 HCAPLUS

DOCUMENT NUMBER: 127:229228

TITLE: A pharmacophore model for PDE IV inhibitors

AUTHOR(S): Polymeropoulos, Emmanuel E.; Hofgen, Norbert

CORPORATE SOURCE: ASTA Medica Group, Department Chemical Research, Frankfurt/Main, D-60314, Germany

SOURCE: Quantitative Structure-Activity Relationships (1997), 16(3), 231-234

CODEN: QSARDI; ISSN: 0931-8771

PUBLISHER: Wiley-VCH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Based on conformational anal. and GRID-contour calcns. we developed a common primary pharmacophore for rolipram analog, nitraquazone and xanthine derivative PDE IV inhibitors. In spite of the structural differences exhibited by the three substance classes we could provide evidence that they share common hydrogen bonding and lipophilic enzyme binding sites.

L19 ANSWER 13 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:374503 HCAPLUS

DOCUMENT NUMBER: 125:104861

TITLE: D-23129: A new anticonvulsant with a broad spectrum activity in animal models of epileptic seizures

AUTHOR(S): Rostock, Angelika; Tober, Christine; Rundfeldt, Chris;

Bartsch, Reni; Engel, Juergen; Polymeropoulos,

Emanuele E.; Kutscher, Bernhard; Loescher,

Wolfgang; Hoenack, Dagmar; et al.

CORPORATE SOURCE: ASTA Medica Group, Department Pharmacology, Radebeul, D-01445, Germany

SOURCE: Epilepsy Research (1996), 23(3), 211-223

CODEN: EPIRE8; ISSN: 0920-1211

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The anticonvulsant activity of the novel drug D-23129 (N-(2-amino-4-(4-fluorobenzylamino)phenyl)carbamic acid Et ester) was evaluated in animal models of epileptic seizures. D-23129 was active after oral and i.p. administration in rats and mice in a range of anticonvulsant tests at nontoxic doses. The compound was active against elec. induced seizures (MES, ED50 rat p.o. = 2.87 mg/kg), against seizures induced chemical by pentylenetetrazole (s.c. PTZ, ED50 mouse p.o. = 13.5 mg/kg), picrotoxin and N-methyl-D-aspartate (NMDA) and in a genetic animal model, the DBA/2 mouse. It was not active against seizures induced by bicuculline and strychnine. Motor impairment, evaluated with the rotarod test and by observation in the open field, was minimal at doses showing anticonvulsant activity. D-23129 was very effective in elevating the threshold for elec. and chemical induced seizures. Considering the dose increasing the MES threshold by 50% (TID50 mouse i.p. = 1.6 mg/kg; TID50 rat i.p. = 0.72 mg/kg) and the TD50 obtained in the rotarod test, the protective index of D-23129 is better than that of valproate and phenytoin. During 14 days chronic oral treatment with 15 mg/kg, no development of tolerance was observed. D-23129 thus presents an orally active, safe, broad spectrum anticonvulsant agent, which is structurally unrelated to anticonvulsants currently used. We expect that D-23129 will improve the treatment of refractory seizures in humans.

L19 ANSWER 14 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:915127 HCAPLUS

DOCUMENT NUMBER: 123:305992

TITLE: Comparative Evaluation of the Predictive Power of Calculation Procedures for Molecular Lipophilicity  
AUTHOR(S): Mannhold, Raimund; Rekker, Roelof F.; Sonntag, Christoph; Ter Laak, Anton M.; Dross, Karl; Polymeropoulos, Emmanuel E.

CORPORATE SOURCE: Department of Lasermedicine, Heinrich-Heine-Universitaet, Duesseldorf, 40225, Germany

SOURCE: Journal of Pharmaceutical Sciences (1995), 84(12), 1410-19

CODEN: JPMSAE; ISSN: 0022-3549

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The predictive power of four calcn. procedures for mol. lipophilicity is checked by comparing with exptl. data (log P and chromatog. RMw) taken from the literature. Two sets of test compds. are used: the first comprises simple organic mols. and the second consists of more complicated drug mols. Our comparative evaluation leads us to conclude that the predictive power is significantly better for not too complicated organic mols. than for drugs with complicated structural pattern. The four investigated calcn. procedures should be arranged in two groups with significantly differing predictive power: (a) Rekker and Hansch/Leo and (b) Ghose/Crippen and Suzuki/Kudo. This conclusion is based on a statistical control using log P and RMw as the independent parameters. Correlations have in common: (1) slopes in correlations with calculated data based on fragmental methods are not significantly different from 1; calcns. with data from atom-based procedures show up in most cases with slopes below 1. (2) The accompanying overall statistics underline the superiority of the fragmental methods. We think that all four tested calcn. procedures have their own restrictions; for future development we would advise a thorough reconsideration of structural effects not fully (or even not at all) incorporated in the data sets. Special attention will have to be paid to the conformational aspects of lipophilic behavior.

L19 ANSWER 15 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:663436 HCAPLUS  
DOCUMENT NUMBER: 121:263436  
TITLE: Chemical and Biological Evaluation of Hydrolysis Products of Cyclophosphamide  
AUTHOR(S): Gilard, Veronique; Martino, Robert; Malet-Martino, Marie-C.; Kutscher, Bernhard; Mueller, Arndt; Niemeyer, Ulf; Pohl, Joerg; Polymeropoulos, Emmanuel E.  
CORPORATE SOURCE: IMRCP Laboratory, Universite Paul Sabatier, Toulouse, 31062, Fr.  
SOURCE: Journal of Medicinal Chemistry (1994), 37(23), 3986-93  
CODEN: JMCMAR; ISSN: 0022-2623  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB <sup>31</sup>P NMR spectroscopy was used to study the products of the decomposition of cyclophosphamide (I) in buffered solns. at pH's ranging between 1.2 and 8.6 at 20° and at pH 7.4 at 37°. At pH 1.2, I undergoes a rapid breakdown (t<sub>1/2</sub> = 1.4 days) of the 2 P-N bonds, giving [HN(CH<sub>2</sub>CH<sub>2</sub>Cl)<sub>2</sub>] and [H<sub>2</sub>N(CH<sub>2</sub>)<sub>3</sub>OP(O)(OH)<sub>2</sub>] as their hydrochlorides. No intermediates were detected. At pH's between 5.4 and 8.6, hydrolysis of I during 17 days led to the sole and previously unknown 9-membered ring compound (II). II resulted from the intramol. alkylation of I giving a bicyclic compound followed by the exothermal cleavage of the P-N bond in the 6-membered ring. At pH values ranging from 3.4 to 8.6, there is little degradation of I since more than 95% of initial I was still present after 7 days at 20°. Under physiol. conditions (pH 7.4, 37°) after 6 days, 45% of I was hydrolyzed (t<sub>1/2</sub> = 6.6 days), leading essentially (30% of initial I) to II. The rate of hydrolysis of II and the nature of its hydrolysis products depended on pH over the range 0-8.6. After a single i.p. injection to mice, II, [H<sub>2</sub>N(CH<sub>2</sub>)<sub>3</sub>OP(O)(OH)<sub>2</sub>], and [Cl(CH<sub>2</sub>)<sub>2</sub>NH(CH<sub>2</sub>)<sub>2</sub>NH(CH<sub>2</sub>)<sub>3</sub>OP(O)(OH)<sub>2</sub>] were less toxic than I. They did not exhibit any direct cytotoxic efficacy on the colony-forming capacity of L1210 cells in vitro, and they had no antitumor activity in vivo against P388 leukemia.

L19 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:569732 HCAPLUS  
DOCUMENT NUMBER: 121:169732  
TITLE: GABAergic activity of triamino-pyridines and triamino-benzenes  
AUTHOR(S): Polymeropoulos, E. E.; Kutscher, B.  
CORPORATE SOURCE: ASTA Med. AG, Frankfurt, 6000, Germany  
SOURCE: Trends QSAR Mol. Modell. 92, Proc. Eur. Symp. Struct.-Act. Relat.: QSAR Mol. Modell., 9th (1993), Meeting Date 1992, 456-60. Editor(s): Wermuth, Camille-Georges. ESCOM: Leiden, Neth.  
CODEN: 59XTAS  
DOCUMENT TYPE: Conference  
LANGUAGE: English

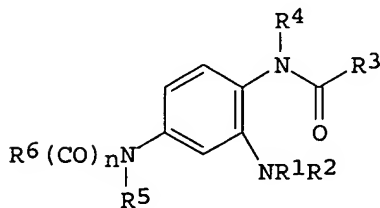
AB Electron d. distribution, isopotential surfaces, and mol. electrostatic potentials were determined for GABA agonists and antagonists. The program GRID was used to evaluate non-covalent drug-receptor interactions. Conformational anal. and structure optimization were also performed.

L19 ANSWER 17 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

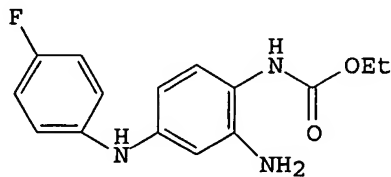
ACCESSION NUMBER: 1993:625705 HCAPLUS  
DOCUMENT NUMBER: 119:225705  
TITLE: 1,2,4-triaminobenzene derivatives and a process for their preparation  
INVENTOR(S): Dieter, Hans Reinhold; Engel, Juergen; Kutscher,

Bernhard; Polymeropoulos, Emmanuel;  
 Szelenyi, Stefan; Nickel, Bernd  
 PATENT ASSIGNEE(S): Asta Medica AG, Germany  
 SOURCE: Ger. Offen., 11 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4200259	A1	19930715	DE 1992-4200259	19920108
EP 554543	A2	19930811	EP 1992-121028	19921210
EP 554543	A3	19931027		
EP 554543	B1	19960228		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
AT 134611	E	19960315	AT 1992-121028	19921210
ES 2084914	T3	19960516	ES 1992-121028	19921210
CA 2086654	AA	19930709	CA 1993-2086654	19930104
CA 2086654	C	20030923		
ZA 9300011	A	19930805	ZA 1993-11	19930104
JP 05345752	A2	19931227	JP 1993-1054	19930107
JP 3145220	B2	20010312		
US 5384330	A	19950124	US 1993-2458	19930108
PRIORITY APPLN. INFO.:			DE 1992-4200259	A 19920108
OTHER SOURCE(S):	CASREACT 119:225705; MARPAT 119:225705			
GI				



I



II

AB The title compds., 2-amino-1,4-bis(acylamino)benzene derivs. I (R1 = hydrogen, alkyl, etc.; R3 = alkoxy, amino, etc.; R4, R5 = hydrogen, alkyl; R6 = arylalkyl) and pharmaceuticals containing them are claimed. I are anticonvulsants, antipyretics, antiepileptics, muscle relaxants, and peripheral analgesics. Some I were tested as antiepileptics in electroshock-induced convulsions in rats. Reductive carbamoylation of 2-amino-4-[(4-fluorobenzy)amino]-1-nitrobenzene gave 2-amino-4-[(4-fluorobenzyl)amino]-1-[(ethoxycarbonyl)amino]benzene [ethyl [2-amino-4-[[[(4-fluorophenyl)methyl]amino]phenyl]carbamate] (II); II dihydrochloride was obtained in 73% yield.

L19 ANSWER 18 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:594860 HCAPLUS

DOCUMENT NUMBER: 119:194860

TITLE: 1-Deprenyl: A unique MAO-B inhibitor

AUTHOR(S): Polymeropoulos, E. E.

CORPORATE SOURCE: Dep. Sci. Inf., ASTA Med. A.-G., Frankfurt/Main, Germany

SOURCE: Inhib. Monoamine Oxidase B (1993), 109-24. Editor(s):

Szelenyi, Istvan. Birkhaeuser: Basel, Switz.  
CODEN: 59HWAP

DOCUMENT TYPE: Conference; General Review  
LANGUAGE: English  
AB A review with 32 refs.

L19 ANSWER 19 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:622766 HCAPLUS

DOCUMENT NUMBER: 115:222766

TITLE: Computer-assisted analysis of the possible binding sites of H1-antagonists

AUTHOR(S): **Polymeropoulos, E. E.**; Kutscher, B.;  
Fleischhauer, I.

CORPORATE SOURCE: ASTA Pharma A.-G., Frankfurt, D-6000/1, Germany  
SOURCE: Pharmacochemistry Library (1991), 16(QSAR: Ration.  
Approaches Des. Bioact. Compd.), 761-4  
CODEN: PHLIDQ; ISSN: 0165-7208

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of antiallergic-antihistaminic compds. acting as H1-receptor antagonists was analyzed with regard to their structural and electronic properties by means of the quantum mech. methods and the program GRID. A model defining possible common binding sites is suggested.

L19 ANSWER 20 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:227015 HCAPLUS

DOCUMENT NUMBER: 108:227015

TITLE: Structure and dynamics of noble gas clusters and cluster ions

AUTHOR(S): Brickmann, J.; **Polymeropoulos, E. E.**;  
Meisel, D.

CORPORATE SOURCE: Tech. Hochsch. Darmstadt, Darmstadt, D-6100, Fed. Rep. Ger.

SOURCE: Contrib. - Symp. At. Surf. Phys. (1986), 342-9.  
Editor(s): Howorka, F.; Lindinger, W.; Maerk, T. D.  
Inst. Atomphys. Univ. Innsbruck: Innsbruck, Austria.  
CODEN: 56GBA4

DOCUMENT TYPE: Conference; General Review

LANGUAGE: English

AB A review with 15 refs. is given of authors own and related work.

L19 ANSWER 21 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:529434 HCAPLUS

DOCUMENT NUMBER: 103:129434

TITLE: Magic numbers in ionized rare-gas clusters

AUTHOR(S): **Polymeropoulos, E. E.**; Brickmann, J.

CORPORATE SOURCE: Inst. Phys. Chemie, Tech. Hochsch. Darmstadt,  
Darmstadt, D-6100, Fed. Rep. Ger.

SOURCE: Surface Science (1985), 156(2), 563-71  
CODEN: SUSCAS; ISSN: 0039-6028

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The relative stability of ionized rare-gas clusters  $X_n^+$ , with  $n = 5-20$  for  $Ar_n^+$  and  $n = 5-26$  for  $Xen^+$  was studied by means of a combined mol. dynamics and Monte Carlo technique. Stable ionized clusters with "magic nos."  $n = 19$  for Ar and  $n = 13, 19$  and  $25$  for Xe occur, in agreement with exptl. time-of-flight mass spectra.

L19 ANSWER 22 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:518290 HCAPLUS

DOCUMENT NUMBER: 103:118290  
 TITLE: Molecular dynamics of ion transport through transmembrane model channels  
 AUTHOR(S): Polymeropoulos, E. E.; Brickmann, J.  
 CORPORATE SOURCE: Inst. Phys. Chem., Tech. Hochsch. Darmstadt, Darmstadt, D-6100, Fed. Rep. Ger.  
 SOURCE: Annual Review of Biophysics and Biophysical Chemistry (1985), 14, 315-30  
 CODEN: ARBCEY; ISSN: 0883-9182  
 DOCUMENT TYPE: Journal; General Review  
 LANGUAGE: English  
 AB A review, with 101 refs., of mol. dynamics of ion transport through transmembrane model channels (i.e., ionophore channels), including the use of simulation methods to describe processes involved in these systems.

L19 ANSWER 23 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1985:442966 HCAPLUS  
 DOCUMENT NUMBER: 103:42966  
 TITLE: The stability of rare gas clusters by ionization  
 AUTHOR(S): Polymeropoulos, E. E.; Loeffler, S.; Brickmann, J.  
 CORPORATE SOURCE: Inst. Phys. Chem., Tech. Hoch. Darmstadt, Darmstadt, D 6100, Fed. Rep. Ger.  
 SOURCE: Zeitschrift fuer Naturforschung, Teil A: Physik, Physikalische Chemie, Kosmophysik (1985), 40A(5), 516-19  
 CODEN: ZTAKDZ; ISSN: 0340-4811  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Computer simulations were made of the dissociation dynamics of Ar and Xe neutral and singly-charged clusters with 5-20 atoms. The stability of clusters with magic nos. (P. and B., 1983) of atoms ( $n = 19$  for Ar, and  $n = 13, 19$  for Xe), as found in time-of-flight mass spectra (J. Farges, et al., 1983), was greater for the ionized clusters than for the neutral clusters, indicating the importance of ionization on the cluster-size distribution found in expts.

L19 ANSWER 24 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1985:442961 HCAPLUS  
 DOCUMENT NUMBER: 103:42961  
 TITLE: Molecular-dynamics simulations in systems of rare gases using Axilrod-Teller and exchange three-atom interactions  
 AUTHOR(S): Polymeropoulos, E. E.; Bopp, P.; Brickmann, J.; Jansen, L.; Block, R.  
 CORPORATE SOURCE: Inst. Phys. Chem., Tech. Hochsch. Darmstadt, Darmstadt, D-6100, Fed. Rep. Ger.  
 SOURCE: Physical Review A: Atomic, Molecular, and Optical Physics (1985), 31(6), 3565-9  
 CODEN: PLRAAN; ISSN: 0556-2791  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB By using previous results (P., et al., 1984), mol.-dynamics simulations of cluster formation in compressed Ar and Xe gases were done with a Lennard-Jones (6,12) potential, Axilrod-Teller 3-atom interactions, and exchange-type interactions. Selective stabilization of the clusters Ar<sub>19</sub>, Xe<sub>13</sub>, and Xe<sub>19</sub> (possibly also Xe<sub>25</sub>) was established, predominantly as a result of the 3-atom exchange potential. These exchange contributions, in combination with selective stability due to cluster ionization, can explain the phenomena observed in existing time-of-flight mass-spectroscopy

expts. on rare-gas-atom clusters.

L19 ANSWER 25 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:144899 HCAPLUS

DOCUMENT NUMBER: 102:144899

TITLE: Solvent effects in ionic transport through transmembrane protein channels

AUTHOR(S): Kappas, U.; Fischer, W.; Polymeropoulos, E. E.; Brickmann, J.

CORPORATE SOURCE: Inst. Phys. Chem., Tech. Hochsch. Darmstadt, Darmstadt, D-1600, Fed. Rep. Ger.

SOURCE: Journal of Theoretical Biology (1985), 112(3), 459-64  
CODEN: JTBIAP; ISSN: 0022-5193

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Ion transport through a gramicidin A-like channel in the presence of solvent mols. with van der Waals parameters of H<sub>2</sub>O was studied by means of mol. dynamics simulation. The presence of solvent mols. in the channel tended to equalize the effective masses of ions through association, thus predicting the exptl. observed ion selectivity of the gramicidin A channel.

L19 ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:119844 HCAPLUS

DOCUMENT NUMBER: 102:119844

TITLE: Exchange perturbation theory calculations of the interaction energy between two ground-state hydrogen atoms

AUTHOR(S): Adams, William H.; Clayton, Meredith M.; Polymeropoulos, E. E.

CORPORATE SOURCE: Dep. Chem., Rutgers Univ., New Brunswick, NJ, 08903, USA

SOURCE: International Journal of Quantum Chemistry, Quantum Chemistry Symposium (1984), 18, 393-406  
CODEN: IJQSDI; ISSN: 0161-3642

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of calcns. were made of the interaction energy between two H atoms in their ground states, using three kinds of exchange perturbation theory. One objective was to test the accuracy that could be achieved with these perturbation methods. A second was to see if the results were consistent with those for H<sub>2</sub><sup>+</sup>. The perturbation equations were solved within the CI approximation, using 226 partially symmetry-contracted, two-electron basis functions. The set of Slater-type basis orbitals was chosen so that we could approx. within 2% the most accurate calculated interaction energies. The second-order energies were reported at a series of nuclear separation and compare them to the best values that have been published. Some of the published values are inaccurate. The % errors in the interaction energies approximated by summing through second and third orders were given.

L19 ANSWER 27 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:577869 HCAPLUS

DOCUMENT NUMBER: 101:177869

TITLE: Analysis of three-body potentials in systems of rare-gas atoms: Axilrod-Teller versus three-atom exchange interactions

AUTHOR(S): Polymeropoulos, E. E.; Brickmann, J.; Jansen, L.; Block, R.

CORPORATE SOURCE: Inst. Phys. Chem., Tech. Hochsch. Darmstadt, Darmstadt, D-6100, Fed. Rep. Ger.



SOURCE: Physical Review A: Atomic, Molecular, and Optical  
Physics (1984), 30(4), 1593-9  
CODEN: PLRAAN; ISSN: 0556-2791

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The triple-dipole (Axilrod-Teller) and the exchange 3-atom potentials were compared for a number of specific arrangements of 3 argon atoms and 3 xenon atoms. For these configurations, total potentials were constructed, taking a Lennard-Jones (6-12) potential for each pair. For all arrangements, the exchange 3-atom potential was the most important correction to the two-body interaction. Qual., the changes with respect to the 2-body potential were more pronounced for Xe than for Ar.

L19 ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:57103 HCAPLUS

DOCUMENT NUMBER: 100:57103

TITLE: The influence of three-body forces on the lifetime and stability of rare gas clusters

AUTHOR(S): Polymeropoulos, E. E.; Brickmann, J.

CORPORATE SOURCE: Inst. Phys. Chem., Tech. Hochsch. Darmstadt,  
Darmstadt, D-6100, Fed. Rep. Ger.

SOURCE: Berichte der Bunsen-Gesellschaft (1983), 87(12),  
1190-5

CODEN: BBPCAX; ISSN: 0005-9021

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The formation of clusters in compressed Ar and Xe gases is studied with the mol. dynamics simulation technique using 2-body Lennard-Jones and 3-body Axilrod-Teller interaction potentials. The effect of 3-body interactions is a function of the temperature of the system and increases with decreasing temperature. The occurrence of clusters corresponding to the "magic-number"  $n = 13$  for Xe is explained in terms of the dispersion forces inherent in the Axilrod-Teller potential. Computer generated images of stable and unstable Xe<sub>13</sub> clusters are presented.

L19 ANSWER 29 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1983:185974 HCAPLUS

DOCUMENT NUMBER: 98:185974

TITLE: On the origin of the occurrence of "magic numbers" in cluster size distributions of xenon in the compressed gas phase

AUTHOR(S): Polymeropoulos, E. E.; Brickmann, J.

CORPORATE SOURCE: Inst. Phys. Chem., Tech. Hochsch. Darmstadt,  
Darmstadt, D-6100, Fed. Rep. Ger.

SOURCE: Chemical Physics Letters (1983), 96(3), 273-5

CODEN: CHPLBC; ISSN: 0009-2614

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The formation of clusters in compressed Ar and Xe is studied with the mol. dynamics simulation technique using 2-body Lennard-Jones and 3-body Axilrod-Teller potentials. The occurrence of clusters corresponding to the "magic number"  $n = 13$  for Xe and the absence of such stable clusters for Ar is due to the dispersion forces that result from triplet-dipole interaction.

L19 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1982:623356 HCAPLUS

DOCUMENT NUMBER: 97:223356

TITLE: Molecular dynamics study of the formation of argon clusters in the compressed gas

AUTHOR(S): Polymeropoulos, E. E.; Brickmann, J.  
 CORPORATE SOURCE: Inst. Phys. Chem., Techn. Hochsch. Darmstadt,  
 Darmstadt, D-6100, Fed. Rep. Ger.  
 SOURCE: Chemical Physics Letters (1982), 92(1), 59-63  
 CODEN: CHPLBC; ISSN: 0009-2614  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The formation of clusters (nucleation) in compressed Ar gas was studied via mol.-dynamics simulation with 2-body Lennard-Jones and 3-body Axilrod-Teller potentials. The 3-body interactions become increasingly important, with decreasing temperature, for cluster stability and cluster size distributions.

L19 ANSWER 31 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1981:93471 HCAPLUS  
 DOCUMENT NUMBER: 94:93471  
 TITLE: Photoinitiated electron transfer between donors and acceptors in monomolecular layer assemblies - EPR and optical studies  
 AUTHOR(S): Cunningham, J.; Polymeropoulos, E. E.;  
 Moebius, D.; Baer, F.  
 CORPORATE SOURCE: Max Planck-Inst. Biophys. Chem., Goettingen, D 3400,  
 Fed. Rep. Ger.  
 SOURCE: NATO Advanced Study Institutes Series, Series C:  
 Mathematical and Physical Sciences (1980), 61(Magn.  
 Reson. Colloid Interface Sci.), 603-8  
 CODEN: NASCD6; ISSN: 0377-2071  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Studies were made by EPR and fluorescence quenching (FQ) techniques of factors influencing photoinitiated electron transfer from donor species organized as one monomol. layer towards acceptor mols. located 20 Å distant in another monomol. layer. Whenever a paraquat type acceptor was incorporated, illumination at wavelengths absorbed by different cyanine or porphyrin donors yielded a weak anisotropic EPR signal consistent with formation of appropriately aligned alkyl-viologen radicals by electron trapping. Time scale and efficiency of EPR signal growth, allied to dependence on thickness of the spacing monolayer, differed markedly from characteristics of FQ. Implications of these differences for relative rates of processes following photoinitiated charge separation in the monolayer assemblies are considered.

L19 ANSWER 32 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1980:642620 HCAPLUS  
 DOCUMENT NUMBER: 93:242620  
 TITLE: Monolayer assemblies with functional units of sensitizing and conducting molecular components: photovoltage, dark conduction and photoconduction in systems with aluminum and barium electrodes  
 AUTHOR(S): Polymeropoulos, E. E.; Moebius, D.; Kuhn, H.  
 CORPORATE SOURCE: Abt. Mol. Systemaufbau, Max-Planck-Inst. Biophys.  
 Chem., Goettingen, D 3400, Fed. Rep. Ger.  
 SOURCE: Thin Solid Films (1980), 68(1), 173-90  
 CODEN: THSFAP; ISSN: 0040-6090  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The vectorial charge separation was studied in assemblies in which a mixed monolayer of an indocarbocyanine dye with the chromophores in the layer plane, a chain-like  $\pi$  electron system oriented perpendicular to the layer plane, and a layer of acceptor mols. were sandwiched between metal

electrodes. The cyanine dye was excited by light, and the excited electron could move via the  $\pi$  electron system and the acceptor to the pos. biased electrode. If these arrangements are sandwiched between metals of very different work functions (Al and Ba), a photovoltage can be measured and is interpreted as being caused by a vectorial electron transfer through the mol. functional unit towards the metal with the smaller work function. The dark conductivity through fatty acid multilayers sandwiched between an Al and a Ba electrode was measured and was interpreted. The hopping of electrons between interlayer states adjacent to the Al electrode is rate-limiting.

L19 ANSWER 33 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1980:224221 HCAPLUS  
 DOCUMENT NUMBER: 92:224221  
 TITLE: Photochromism in monolayers  
 AUTHOR(S): Polymeropoulos, E. E.; Moebius, D.  
 CORPORATE SOURCE: Abt. Mol. Systemaufbau, Max-Planck-Inst. Biophys.  
 Chem., Goettingen, D-3400, Fed. Rep. Ger.  
 SOURCE: Berichte der Bunsen-Gesellschaft (1979), 83(12),  
 1215-22  
 CODEN: BBPCAX; ISSN: 0005-9021  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The photochromic properties of 1'-octadecyl-3',3'-dimethyl-6-nitropiro[2H-1-benzopyran-2,2'-indoline](I) were studied in monolayers at the air-H<sub>2</sub>O interface by measuring the surface pressure-area isotherms and the surface potential of several mixts. of I with tripalmitine. By using the Langmuir-Blodgett technique, mixed monolayers of tripalmitine and I in a molar mixing ratio of 6:1 were transferred onto glass slides and their photochromic properties in monolayer assemblies were studied.

L19 ANSWER 34 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1980:203868 HCAPLUS  
 DOCUMENT NUMBER: 92:203868  
 TITLE: Exchange perturbation theory. IV. Calculations on diatomic hydrogen (H) ion  
 AUTHOR(S): Adams, William H.; Polymeropoulos, E. E.  
 CORPORATE SOURCE: Dep. Chem., Rutgers, State Univ., New Brunswick, NJ,  
 08903, USA  
 SOURCE: Journal of Chemical Physics (1980), 72(5), 2981-9  
 CODEN: JCPSA6; ISSN: 0021-9606  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Authors have applied the two localized-wave-functions (LW) exchange-perturbation-theories (EPT) which they have proposed (1978) to the 1s $\sigma$  and 2p $\sigma$  states of H<sub>2</sub><sup>+</sup> with the objective of verifying the insights gained from these EPT's and testing their accuracy. The one LW EPT detcs. a primitive wave function identical to that of the Eisenschitz-London EPT through first order, but which differs from it in all higher orders. The other detcs. a function identical to that of the Hirschfelder-Silbey EPT through first order and through infinite order, but which differs from it through all intermediate orders. In terms of the perturbation expansion of the interaction energy through third order, authors' EPT's are as accurate as the original EPT's to which they are related. The LW EPT's have the conceptual asset that their primitive wave functions are least distorted from the zero order wave function in a precisely defined sense. Interaction energies were also calculated using the integrals which define the interaction energies in terms of LW's, and substituting the LW's approximated by sums through first, second, and third order. The energies generally increase in accuracy as the LW is

summed to higher orders. When each order contribution to the LW is multiplied by a weight which is determined to minimize the interaction energy, and

the LW is summed through third order, the interaction energy is in error by 0.07% or less for nuclear sepns. ranging from 1.0 to 10.0 bohr. An examination of the LW's shows how the optimization procedure works. Other quantities are calculated which show that the LW EPT's are systematically refinable methods for the calcn. of LW's as well as for the calcn. of interaction energies. This is important because LW'S may be used to calculate distinct "phys." contributions to interaction energies.

L19 ANSWER 35 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1979:131519 HCAPLUS

DOCUMENT NUMBER: 90:131519

TITLE: Electron tunneling through superconducting aluminum/monolayer/lead junctions

AUTHOR(S): Polymeropoulos, E. E.

CORPORATE SOURCE: Abt. Mol. Syst., Mas-Planck-Inst. Biophys. Chem., Goettingen, Fed. Rep. Ger.

SOURCE: Solid State Communications (1978), 28(10), 883-5  
CODEN: SSCO4; ISSN: 0038-1098

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The current-voltage characteristics of Al/adsorbed monolayer/Pb junctions was determined at 77, 4.2, and 1.8 K for applied voltages 1-3 mV. At 77 K the current changes linearly with voltage whereas at 4.2 and 1.8 K the relation becomes nonlinear. Based on results at 1.8 K, an approx. band gap for Pb equal to 2.6 meV was obtained. The observation of a nonlinear current-voltage characteristic at temps. where Pb becomes superconducting is strong evidence that the observed current through the insulator is a tunneling current.

L19 ANSWER 36 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1978:589545 HCAPLUS

DOCUMENT NUMBER: 89:189545

TITLE: Electrical conduction through adsorbed monolayers

AUTHOR(S): Polymeropoulos, E. E.; Sagiv, J.

CORPORATE SOURCE: Abt. Mol. Systemaufbau, Max-Planck-Inst. Biophys. Chem., Goettingen, Fed. Rep. Ger.

SOURCE: Journal of Chemical Physics (1978), 69(5), 1836-47  
CODEN: JCPSA6; ISSN: 0021-9606

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Elec. conduction was studied in Al/adsorbed monolayer/Al junctions. The adsorbed monolayers were long chain saturated fatty acids (23-14 C atom chain), short chain perfluorinated fatty acids (10-7 C atom chain), and n-octadecyltrichlorosilane. The current observed decreased rapidly with decreasing temperature from 295 K to .apprx.77 K at which point the decrease in current with decreasing temperature became very small. At room temperature (295 K)

there was no definite relation between the d.c. conductivity and the length of the fatty acids. At  $\leq 77$  K, however, the d.c. conductivity was exponentially dependent on the fatty-acid chain length. Thus, at  $\leq 77$  K the conduction mech. is tunneling through the monolayer. The tunneling barrier height was of the order of 2.8 and 5.2 eV for fatty acids and perfluorinated fatty acids, resp. By artificially producing mol. holes in monolayers, in the presence of such holds it was shown, the current increases by at least one order of magnitude while the effective barrier height is lowered by 10%. Differences between the present results and those previously obtained with monolayers deposited from an air-water

interface (Langmuir-Blodgett monolayer) are discussed.

L19 ANSWER 37 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1978:569628 HCAPLUS

DOCUMENT NUMBER: 89:169628

TITLE: Adsorbed monolayers. Molecular organization and electrical properties

AUTHOR(S): Sagiv, J.; Polymeropoulos, E. E.

CORPORATE SOURCE: Max-Planck-Inst. Biophys. Chem., Karl-Friedrich-Bonhoeffer-Inst., Goettingen-Nikolausberg, Fed. Rep. Ger.

SOURCE: Berichte der Bunsen-Gesellschaft (1978), 82(9), 882  
CODEN: BBPCAX; ISSN: 0005-9021

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Adsorption was used to obtain monolayers with a controllable mol. organization. The adsorption process and structure of dye-containing monolayers were studied by spectroscopy. Adsorbed monolayers were used in study of elec. conductivity through organic films. Oleophobic monolayers of long-chain surfactants and mixed monolayers containing dyes were studied. Octadecyltrichlorosilane (OTS) was used as an adsorbate-adsorbent bonding agent. Mol-holes were produced in OTS + dye monolayers by removal of the dye. Addition of other mols. to those holes gives a type of mol. organization. Anisotropic mol. distributions were induced in monolayers by adsorption on oriented polymeric surfaces. The elec. properties (capacitance, current, tunneling, and dielec. constant) were studied of adsorbed monolayers on Al electrodes. These adsorbed monolayers included fatty acids, perfluorinated fatty acids, and OTS. Adsorbed monolayers may be used as insulators in Al/monolayer Pb superconducting tunneling junctions.

L19 ANSWER 38 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1978:435174 HCAPLUS

DOCUMENT NUMBER: 89:35174

TITLE: Photoconduction in monolayer assemblies with functional units of sensitizing and conducting molecular components

AUTHOR(S): Polymeropoulos, E. E.; Moebius, D.; Kuhn, H.

CORPORATE SOURCE: Abt. Mol. Systemaufbau, Max-Planck-Inst. Biophys. Chem., Goettingen, Fed. Rep. Ger.

SOURCE: Journal of Chemical Physics (1978), 68(8), 3918-31  
CODEN: JCPSA6; ISSN: 0021-9606

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Vectorial charge separation was studied in assemblies where a mixed monolayer of a cyanine dye with the chromophores in the layer plane and a chainlike  $\pi$ -electron system oriented perpendicular to the layer plane are sandwiched between fatty acid monolayers and metal electrodes. The cyanine dye is excited by light, and the excited electrons move through the  $\pi$ -electron system which acts as the conducting element. Conduction takes place according to different mechanisms depending on the temperature. In the low-temperature mode the logarithm of the photocurrent decreases linearly with  $(1/T)^{1/2}$ , while in the high-temperature mode it decreases linearly with  $1/T$ ; in both modes the photocurrent is proportional to the light intensity and its logarithm increases linearly with the bias voltage. If the conducting  $\pi$ -electron system is absent, the photocurrent is about an order of magnitude smaller but again proportional to the light intensity. Its logarithm increases linearly with the square root of the bias voltage. The results in the complex assembly can be interpreted by assuming that the excited electron is transferred from the cyanine dye to the

$\pi$ -electron system by tunneling or by thermal activation over a barrier of 0.25 eV; from there it tunnels through the next fatty acid layer to an interface state, and then hops to the pos. biased electrode. This model can be checked by specifically altering the thickness of the tunneling barrier (by exchanging arachidic acid for fatty acids with shorter chain lengths). In the arrangement where the conducting element is absent, the results are interpreted by assuming that the excited electron either tunnels through or is thermally activated over the potential barrier of the hydrocarbon matrix (1 eV). The different voltage dependence in the two arrangements with and without the conducting  $\pi$ -electron system can be quant. explained as being due to the fact that the chromophore of the cyanine dye is perpendicular to the applied field, while the chain of the  $\pi$ -electron system is parallel to this field.

L19 ANSWER 39 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1978:126608 HCAPLUS

DOCUMENT NUMBER: 88:126608

TITLE: Exchange perturbation theory. III.  
Hirschfelder-Silbey type

AUTHOR(S): Polymeropoulos, E. E.; Adams, William H.

CORPORATE SOURCE: Sch. Chem., Rutgers, State Univ., New Brunswick, NJ,  
USA

SOURCE: Physical Review A: Atomic, Molecular, and Optical  
Physics (1978), 17(1), 24-9  
CODEN: PLRAAN; ISSN: 0556-2791

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An exchange perturbation theory is developed which yields in infinite order the same primitive function  $F$  that is found in infinite order with the Hirschfelder-Silbey (HS) theory. The perturbation equations are identical to the HS equations only through first order. This is because the perturbing potential in our theory is not the bare interaction potential of the HS theory, but rather that potential screened by a nonlocal potential. The screening is the weakest that we have found in studying the equations satisfied by primitive functions, which are least distorted from products of the functions for the subsystems when the interactions have been turned off. It is argued that this HS-type theory is best used when the interactions are weak.

L19 ANSWER 40 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1978:126607 HCAPLUS

DOCUMENT NUMBER: 88:126607

TITLE: Exchange perturbation theory. II. Eisenschitz-London  
type

AUTHOR(S): Polymeropoulos, E. E.; Adams, William H.

CORPORATE SOURCE: Sch. Chem., Rutgers, State Univ., New Brunswick, NJ,  
USA

SOURCE: Physical Review A: Atomic, Molecular, and Optical  
Physics (1978), 17(1), 18-23  
CODEN: PLRAAN; ISSN: 0556-2791

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An exchange perturbation theory is developed which is identical through first order in the primitive function  $G$  with the Eisenschitz-London (EL) theory. In higher orders,  $G$  is different from the EL primitive function and from the primitive functions of related theories. The function  $G$  is least distorted from the zeroth-order function  $F_0$ , a product of functions for the subsystems when the interactions have been set equal to zero. The potential which distorts  $F_0$  into  $G$  is more thoroughly screened than in any other theory we have examined. This EL-type theory should be used when the

unscreened interactions are strong.

L19 ANSWER 41 OF 41 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1978:126606 HCAPLUS

DOCUMENT NUMBER: 88:126606

TITLE: Exchange perturbation theory. I. General definitions and relations

AUTHOR(S): Adams, William H.; Polymeropoulos, E. E.

CORPORATE SOURCE: Sch. Chem., Rutgers, State Univ., New Brunswick, NJ, USA

SOURCE: Physical Review A: Atomic, Molecular, and Optical Physics (1978), 17(1), 11-17

CODEN: PLRAAN; ISSN: 0556-2791

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A class of primitive functions are defined which are least distorted from the unsymmetrized function  $F_0$ , a product of atomic or other group functions, in the limit that the interactions between the groups have been turned off. These primitive functions have the property that at least one Schrodinger eigenfunction may be obtained from them by sym. projection. The screened potential is regarded as a perturbation and the corresponding Rayleigh-Schrodinger perturbation equations are derived. It is shown that a number of inequivalent, but equally valid energy expressions may be defined in terms of the primitive functions. Only when the primitive function is calculated exactly to infinite order will the different energy expressions all yield the same numerical value. It is suggested that this provides a check on the accuracy of approx. primitive functions.

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L5 STR

L7 118852 SEA FILE=REGISTRY SSS FUL L5

L8 STR

L9 157 SEA FILE=REGISTRY SUB=L7 SSS FUL L8

L10 STR

L11 18 SEA FILE=REGISTRY SUB=L9 SSS FUL L10

L12 7 SEA FILE=HCAPLUS ABB=ON PLU=ON L11

L15 43 SEA FILE=HCAPLUS ABB=ON PLU=ON ("EMIG P"/AU OR "EMIG PETER"/AU)

L16 41 SEA FILE=HCAPLUS ABB=ON PLU=ON L15 NOT L12

L17 67 SEA FILE=HCAPLUS ABB=ON PLU=ON ("GUNTHER E"/AU OR "GUNTHER ECKHARD"/AU) NOT (L12 OR L16)

L18 1 SEA FILE=HCAPLUS ABB=ON PLU=ON (("AUE B J"/AU OR "AUE BEATE"/AU)) NOT (L12 OR L16 OR L17)

L19 41 SEA FILE=HCAPLUS ABB=ON PLU=ON (("POLYMEROPOULOS E"/AU OR "POLYMEROPOULOS E E"/AU OR "POLYMEROPOULOS EMANUELE E"/AU OR "POLYMEROPOULOS EMMANUEL"/AU OR "POLYMEROPOULOS EMMANUEL E"/AU)) NOT (L12 OR L16 OR L17 OR L18)

L20 12 SEA FILE=HCAPLUS ABB=ON PLU=ON (("BAASNER S"/AU OR "BAASNER SIIKE"/AU OR "BAASNER SILKE"/AU)) NOT (L12 OR L16 OR L17 OR L18 OR L19)

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L20 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:1261687 HCAPLUS

DOCUMENT NUMBER: 144:22948

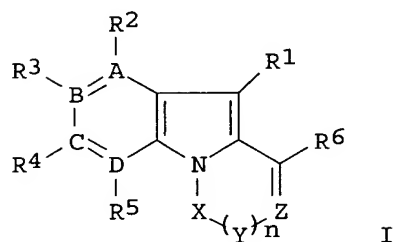
TITLE: Preparation of fused indoles as anticancer drugs.

INVENTOR(S): Weinberger, Heinz; Beckers, Thomas; Schmidt, Mathias;

**Baasner, Silke; Nickel, Bernd**  
 PATENT ASSIGNEE(S): Zentaris AG, Germany; Zentaris GmbH  
 SOURCE: U.S. Pat. Appl. Publ., 47 pp., Cont.-in-part of U.S. Ser. No. 233,135.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005267303	A1	20051201	US 2005-136688	20050524
US 2004039197	A1	20040226	US 2002-233135	20020830
PRIORITY APPLN. INFO.:			US 2001-317102P	P 20010904
			US 2002-233135	A2 20020830
			DE 2001-10143079	A 20010903

OTHER SOURCE(S): MARPAT 144:22948  
 GI



AB The invention relates to novel, substituted, fused indole and heteroindole derivs. of the general formula I their tautomers, stereoisomers, mixts. and pharmaceutically acceptable salts, their synthesis and their use as pharmaceuticals, especially as anti-tumor agents, for mammals, especially for man.

Title compds. [I; R1 = H, (substituted) aryl, heteroaryl, cycloalkyl, alkyl; A, B, D, E = substituted C; R2-R5 = H, halo, cyano, NO<sub>2</sub>, OH, alkyl, haloalkyl, alkoxy, haloalkoxy, alkylcarbonyloxy, alkylsulfonyl, CO<sub>2</sub>H, amino, etc.; R6 = (substituted) aryl, heteroaryl, cycloalkyl, alkyl, alkoxy; X = CO; n = 0 ], were prepared Thus, reaction of 1H-indole-2-ylmethanone oxime Ph methanone oxime (preparation given) with carbonyldiimidazole in refluxing THF gave (5-methoxy-1H-indole-2-yl)phenylmethanone oxime. This at 3.16 µg/mL showed 90.7% antiproliferative activity against HeLa/KB in an XTT cytotoxicity test.

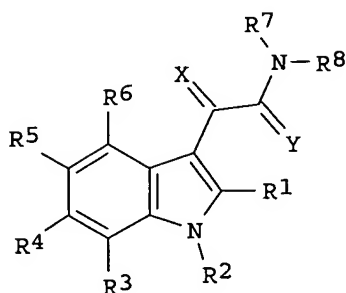
L20 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:141028 HCAPLUS  
 DOCUMENT NUMBER: 142:240315  
 TITLE: Preparation of indolyl-3-glyoxylic acid amides for the treatment of tumors  
 INVENTOR(S): Gerlach, Matthias; Schuster, Tilmann; Schmidt, Peter; Baasner, Silke; Guenther, Eckhard  
 PATENT ASSIGNEE(S): Zentaris G.m.b.H., Germany  
 SOURCE: PCT Int. Appl., 25 pp.  
 CODEN: PIXXD2

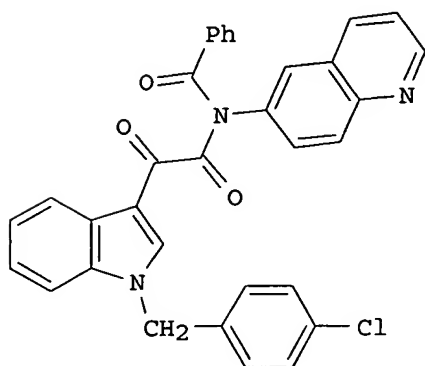


DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005014542	A2	20050217	WO 2004-EP7573	20040709
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10334040	A1	20050310	DE 2003-10334040	20030725
PRIORITY APPLN. INFO.:			DE 2003-10334040	A 20030725
GI				



I



II

AB Title compds. I [R1, R3, R4, R5, R6 = H, (un)substituted alkyl, cycloalkyl, aryl, etc.; R7 = SO2X1, COX2, COOX3, etc.; X1 = N(alkyl)2, OH, (un)substituted alkyl, etc.; X2 = (un)substituted aryl, heteroaryl, alkylaryl, etc.; X3 = (un)substituted cycloalkyl, heterocyclyl, aryl, etc.; R8 = Het; X = O, S with provisos; Y = O, S] and their

pharmaceutically acceptable salts were prepared. In human cervical cancer cell line (KB/HeLa) antiproliferative assay, indolylglyoxylic acid amide II exhibited an IC<sub>50</sub> value of 0.170 µg/mL. Compds. I are claimed to be useful for the treatment of tumors.

L20 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:885644 HCAPLUS

DOCUMENT NUMBER: 140:26268

TITLE: Switching Off HER-2/neu in a Tetracycline-Controlled Mouse Tumor Model Leads to Apoptosis and Tumor-Size-Dependent Remission

AUTHOR(S): Schiffer, Ilka B.; Gebhard, Susanne; Heimerdinger, Carolin K.; Heling, Annette; Hast, Jochem; Wollscheid, Ursula; Seliger, Barbara; Tanner, Berno; Gilbert, Sandra; Beckers, Thomas; Baasner, Silke; Brenner, Walburgis; Spangenberg, Christian; Prawitt, Dirk; Trost, Tatjana; Schreiber, Wolfgang G.; Zabel, Bernhard; Thelen, Manfred; Lehr, Hans-Anton; Oesch, Franz; Hengstler, Jan G.

CORPORATE SOURCE: Departments of Radiology, Institute of Toxicology, University of Mainz, Mainz, 55131, Germany

SOURCE: Cancer Research (2003), 63(21), 7221-7231

CODEN: CNREA8; ISSN: 0008-5472

PUBLISHER: American Association for Cancer Research

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Overexpression of the receptor tyrosine kinase HER-2/neu is associated with poor prognosis in patients with breast and ovarian cancer. Recent excitement has surrounded the therapeutic effects of HER-2-blocking therapy strategies and has rekindled interest on the mol. mechanisms of HER-2/neu in tumor biol. To study the role of HER-2/neu overexpression in vivo, the authors used a murine fibroblast cell line (NIH3T3-her2) conditionally expressing human HER-2/neu under control of a tetracycline-responsive promoter. Expression of HER-2 could be down-regulated below detection limit (>625-fold dilution) by exposure of NIH3T3-her2 cells to anhydrotetracycline (ATc). S.c. injection of NIH3T3-her2 cells into nude mice resulted in rapid tumor growth. Mice with mean tumor vols. of 0.2, 0.8, 1.9, and 14.9 cm<sup>3</sup> were treated daily with 10 mg/kg ATc to switch off HER-2/neu expression, producing redns. in tumor size of 100, 98.1, 81.4, and 74.2%, resp., by 7 days after onset of ATc administration. Different long-term effects of HER-2 down-regulation were observed when mice with small (0.2 cm<sup>3</sup>), intermediate (0.8-1.2 cm<sup>3</sup>) and large (≥1.9 cm<sup>3</sup>) tumors received ATc for up to 40 days. Complete remission was observed for 100, 40, and 18% of the small-, intermediate-, and large-sized tumors, resp. However, after 20-45 days of ATc administration, recurrent tumor growth was observed for all mice, even in those with previous complete remissions. The time periods for which mean tumor volume could be suppressed to vols. <0.1 cm<sup>3</sup> under ATc administration were 34, 22, 8, and 0 days for tumors with initial vols. of 0.2, 0.8, 1.9 and 14.9 cm<sup>3</sup>, resp. Interestingly, HER-2 remained below the detection limit in recurrent tumor tissue, suggesting that initially HER-2-dependent tumors switched to HER-2 independence. The "second hits" leading to HER-2-independent tumor growth have not yet been identified. The rapid regression of tumors after down-regulation of HER-2 was explained by two independent mechanisms: (a) a block in cell cycle progression, as evidenced by a decrease in Ki-67 antigen expression from 40% before ATc treatment to 8.3% after 7 days of ATc treatment; and (b) induction of apoptosis as demonstrated by caspase-3 activation and by the terminal deoxynucleotidyltransferase (Tdt)-mediated nick end labeling assay (TUNEL). In conclusion, the authors have shown that switching off HER-2

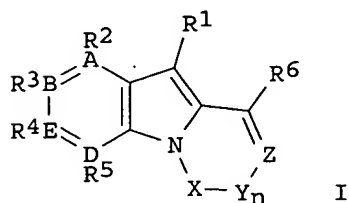
may disturb the sensitive balance between cell proliferation and cell death, leading to apoptosis and tumor remission. Tumor remission was dependent on the volume of the tumors before down-regulation of HER-2/neu.

REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:202649 HCAPLUS  
 DOCUMENT NUMBER: 138:238205  
 TITLE: Preparation of fused indoles as anticancer drugs.  
 INVENTOR(S): Weinberger, Heinz; Beckers, Thomas; Schmidt, Mathias; Baasner, Silke; Nickel, Bernd  
 PATENT ASSIGNEE(S): Zentaris A.-G., Germany  
 SOURCE: PCT Int. Appl., 118 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003020731	A1	20030313	WO 2002-EP9539	20020827
W: AU, BG, BR, BY, CA, CN, CO, CZ, EE, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LT, LV, MK, MX, NO, NZ, PH, PL, RO, RU, SG, SI, SK, UA, UZ, YU, ZA, AM, AZ, MD, TJ, TM				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR				
DE 10143079	A1	20030515	DE 2001-10143079	20010903
CA 2458399	AA	20030313	CA 2002-2458399	20020827
EP 1423393	A1	20040602	EP 2002-767436	20020827
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002012300	A	20041013	BR 2002-12300	20020827
CN 1551885	A	20041201	CN 2002-817263	20020827
NZ 531642	A	20050128	NZ 2002-531642	20020827
JP 2005508898	T2	20050407	JP 2003-525001	20020827
ZA 2004001290	A	20040323	ZA 2004-1290	20040218
NO 2004000831	A	20040413	NO 2004-831	20040225
PRIORITY APPLN. INFO.:			DE 2001-10143079	A 20010903
			WO 2002-EP9539	W 20020827
OTHER SOURCE(S):			MARPAT 138:238205	
GI				



AB Title compds. [I; R1 = H, (substituted) aryl, heteroaryl, cycloalkyl, alkyl; A, B, D, E = C, N; R2-R5 = electron pair, H, halo, cyano, NO<sub>2</sub>, OH, alkyl, haloalkyl, alkoxy, haloalkoxy, alkylcarbonyloxy, alkylsulfonyl, CO<sub>2</sub>H, amino, etc.; R6, R7, R8 = (substituted) aryl, heteroaryl, cycloalkyl, alkyl; X = CO, SO, SO<sub>2</sub>; Y = O, NR<sub>7</sub>; n = 0, 1; Z = CR<sub>8</sub>], were

prepared Thus, reaction of (5-methoxy-1H-indol-2-yl) Ph methanone oxime (preparation given) with carbonyldiimidazole in refluxing THF gave 5-methoxy-3-phenyl-1,2,5-oxadiazino[4,5-a]indol-6-one. This at 3.16 µg/mL showed 90.7% antiproliferative activity against HeLa/KB in an XTT cytotoxicity test.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:80889 HCAPLUS

DOCUMENT NUMBER: 136:272658

TITLE: Bis(1H-2-indolyl)methanones as a Novel Class of Inhibitors of the Platelet-Derived Growth Factor Receptor Kinase

AUTHOR(S): Mahboobi, Siavosh; Teller, Steffen; Pongratz, Herwig; Hufsky, Harald; Sellmer, Andreas; Botzki, Alexander; Uecker, Andrea; Beckers, Thomas; Baasner, Silke; Schaechtele, Christoph; Ueberall, Florian; Kassack, Matthias U.; Dove, Stefan; Boehmer, Frank-D.

CORPORATE SOURCE: Faculty of Chemistry and Pharmacy, Institute of Pharmacy, University of Regensburg, Regensburg, D-93040, Germany

SOURCE: Journal of Medicinal Chemistry (2002), 45(5), 1002-1018

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:272658

AB The novel lead bis(1H-2-indolyl)methanone inhibits autophosphorylation of platelet-derived growth factor (PDGF) receptor tyrosine kinase in intact cells. Various substituents in the 5- or 6-position of one indole ring increase or preserve potency, whereas most modifications of the ring structures and of the methanone group as well as substitution at both indoles result in weak or no activity. An ATP binding site model, derived by homol. from the FGFR-1 tyrosine kinase crystal structure suggesting hydrogen bonds of one indole NH and the methanone oxygen with the backbone carbonyl and amide, resp., of Cys684, explains why only one indole moiety is open for substitution and locates groups in the 5- or 6-position outside the pocket. Some of the most active derivs., inhibit both isoforms of the PDGF receptor kinase in intact cells, with IC<sub>50</sub> of 0.1-0.3 µM, and purified PDGFβ-receptor in vitro, with IC<sub>50</sub> of 0.09, 0.1, or 0.02 µM, resp. PDGF-stimulated DNA synthesis is inhibited by these derivs. with IC<sub>50</sub> values of 1-3 µM. Kinetic anal. of one compound showed an ATP-competitive mode of inhibition. The compds. are inactive or weakly active toward a number of other tyrosine kinases, including the FGF receptor 1, EGF receptor, and c-Src kinase, as well as toward serine-threonine kinases, including different PKC isoforms and GRK2, and appear therefore selective for PDGF receptor inhibition.

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:836852 HCAPLUS

DOCUMENT NUMBER: 136:112229

TITLE: Synthetic 2-Aroylindole Derivatives as a New Class of Potent Tubulin-Inhibitory, Antimitotic Agents

AUTHOR(S): Mahboobi, Siavosh; Pongratz, Herwig; Hufsky, Harald; Hockemeyer, Joerg; Frieser, Markus; Lyssenko, Alexei; Paper, Dietrich H.; Buergermeister, Jutta; Boehmer,

CORPORATE SOURCE: Frank-D.; Fiebig, Heinz-Herbert; Burger, Angelika M.;  
Baasner, Silke; Beckers, Thomas  
Faculty of Chemistry and Pharmacy Institute of  
Pharmacy, University of Regensburg, Regensburg,  
D-93040, Germany

SOURCE: Journal of Medicinal Chemistry (2001), 44(26),  
4535-4553  
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:112229

AB A new class of simple synthetic antimitotic compds. based on  
2-aryloindoles was discovered. (5-Methoxy-1H-2-indolyl)-phenylmethanone  
(I) as well as analogous 3-fluorophenyl- and 3-methoxyphenyl derivs.  
displayed high cytotoxicity of IC<sub>50</sub> = 20 to 75 nM against the human  
HeLa/KB cervical, SK-OV-3 ovarian, and U373 astrocytoma carcinoma cell  
lines. The inhibition of proliferation correlated with the arrest in the  
G2/M phase of the cell cycle. In in vitro assays with tubulin isolated  
from bovine brain, in general antiproliferative activity correlated with  
inhibition of tubulin polymerization. Thus, the antimitotic activity of  
2-aryloindoles is explained by interference with the mitotic spindle apparatus  
and destabilization of microtubules. In contrast to colchicine,  
vincristine, nocodazole, or taxol, I did not significantly affect the  
GTPase activity of  $\beta$ -tubulin. Interestingly, selected compds.  
inhibited angiogenesis in the chorioallantoic membrane (CAM) assay. In  
xenograft expts., I was highly active after oral administration at 200  
mg/kg against the human amelanocytic melanoma MEXF 989 in athymic nude  
mice. We conclude, that 2-aryloindoles constitute an interesting new  
class of antitubulin agents with the potential to be clin. developed for  
cancer treatment.

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:816437 HCAPLUS

DOCUMENT NUMBER: 135:352771

TITLE: (Hetero)indole derivatives, their preparation,  
pharmaceutical compositions, and their use as  
antitumor agents

INVENTOR(S): Beckers, Thomas; Baasner, Silke; Klenner,  
Thomas; Mahboobi, Siavosh; Pongratz, Herwig; Frieser,  
Markus; Hufsky, Harald; Hockemeyer, Jorg; Fiebig,  
Heinz-Herbert; Burger, Angelika; Bohmer, Frank-D.

PATENT ASSIGNEE(S): Asta Medica A.-G., Germany

SOURCE: PCT Int. Appl., 89 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001082909	A2	20011108	WO 2001-EP4783	20010427
WO 2001082909	A3	20020314		
W:	AT, AU, BG, BR, BY, CA, CH, CN, CO, CZ, DE, DK, DZ, EE, ES, FI, GB, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LT, LU, LV, MK, MX, NO, NZ, PL, PT, RO, RU, SE, SG, SI, SK, TR, UA, US, UZ, YU, ZA, AM, AZ, MD, TJ, TM			

RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,  
PT, SE, TR

DE 10020852	A1	20011031	DE 2000-10020852	20000428
DE 10102629	A1	20020725	DE 2001-10102629	20010120
CA 2407677	AA	20021028	CA 2001-2407677	20010427
EP 1276720	A2	20030122	EP 2001-947247	20010427

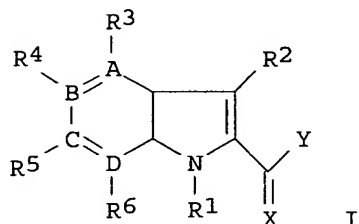
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IE, SI, LT, LV, FI, RO, MK, CY, TR

BR 2001010414	A	20030211	BR 2001-10414	20010427
JP 2004501092	T2	20040115	JP 2001-579784	20010427
EE 200200607	A	20040415	EE 2002-607	20010427
AU 783459	B2	20051027	AU 2001-68984	20010427
NO 2002005150	A	20021216	NO 2002-5150	20021025
BG 107309	A	20030930	BG 2002-107309	20021125

PRIORITY APPLN. INFO.:

DE 2000-10020852	A	20000428
DE 2001-10102629	A	20010120
WO 2001-EP4783	W	20010427

OTHER SOURCE(S): CASREACT 135:352771; MARPAT 135:352771  
GI



AB The invention discloses indole and heteroindole derivs. I [R1 = H, C1-6 alkyl, C1-6 alkylcarbonyl, etc.; R2 = H, halo, cyano, etc.; R3-R6 = H, halo, nitro, etc.; A-D = C, N; Y = (un)substituted C6-14 aryl, etc.; X = O, S, NH, CHOH], and tautomers, stereoisomers, mixts. and salts thereof, as well as the production thereof and the use thereof for the treatment of tumors.

L20 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:795073 HCAPLUS

DOCUMENT NUMBER: 135:331343

TITLE: Preparation of 1H-indol-2-yl aryl ketones and related compounds as antitumor agents

INVENTOR(S): Beckers, Thomas; **Baasner, Silke**; Klenner, Thomas; Mahboobi, Siavosh; Pongratz, Herwig; Frieser, Markus; Hufsky, Harald; Hockemeyer, Joerg; Fiebig, Heinz-Herbert; Burger, Angelika; Boehmer, Frank-D.

PATENT ASSIGNEE(S): Asta Medica A.-G., Germany

SOURCE: Ger. Offen., 34 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

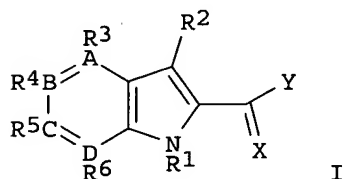
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DE 10020852	A1	20011031	DE 2000-10020852	20000428
WO 2001082909	A2	20011108	WO 2001-EP4783	20010427

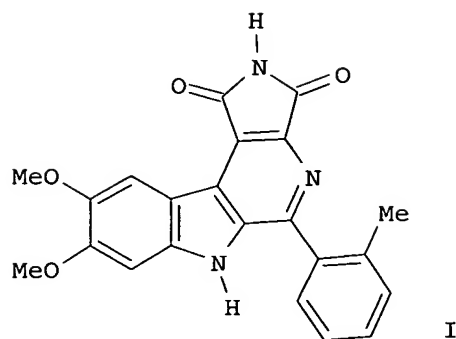
WO 2001082909 A3 20020314  
W: AT, AU, BG, BR, BY, CA, CH, CN, CO, CZ, DE, DK, DZ, EE, ES, FI, GB, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LT, LU, LV, MK, MX, NO, NZ, PL, PT, RO, RU, SE, SG, SI, SK, TR, UA, US, UZ, YU, ZA, AM, AZ, MD, TJ, TM  
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR  
US 2002091124 A1 20020711 US 2001-843139 20010427  
CA 2407677 AA 20021028 CA 2001-2407677 20010427  
EP 1276720 A2 20030122 EP 2001-947247 20010427  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, TR  
BR 2001010414 A 20030211 BR 2001-10414 20010427  
JP 2004501092 T2 20040115 JP 2001-579784 20010427  
EE 200200607 A 20040415 EE 2002-607 20010427  
US 2003158216 A1 20030821 US 2002-279123 20021024  
US 2003158216 A1 20030821 US 2002-279123 20021024  
NO 2002005150 A 20021216 NO 2002-5150 20021025  
ZA 2002009137 A 20040618 ZA 2002-9137 20021111  
BG 107309 A 20030930 BG 2002-107309 20021125  
PRIORITY APPLN. INFO.: DE 2000-10020852 A 20000428  
DE 2001-10102629 A 20010120  
US 2001-843139 B1 20010427  
WO 2001-EP4783 W 20010427  
OTHER SOURCE(S): MARPAT 135:331343  
GI



AB Use of title compds. [I; R1 = H, alkylcarbonyl, alkylaminoalkyl, dialkylaminoalkyl, (hetero)cyclyl; R2 = H, halo, cyano, NO<sub>2</sub>, (substituted) alkyl, alkoxy, etc.; A-D = N, (substituted) C; R3-R6 = free electron pair if A-D = N, or H, halo, cyano, NO<sub>2</sub>, alkyl, etc. if A-D = C; Y = (substituted) aryl; X = O, S, NH, (H,OH)], for preparation of drugs for treatment of tumor illness in mammals is claimed. Thus, 5-methoxy-1H-indol-2-yl Ph ketone (general preparation given) showed antitumor activity with IC<sub>50</sub> = 96.5 nM in rat glioma cell lines C6.

L20 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 2000:398021 HCAPLUS  
DOCUMENT NUMBER: 133:164199  
TITLE: Pyrrolo[3,4-c]-β-carboline-diones as a novel class of inhibitors of the platelet-derived growth factor receptor kinase  
AUTHOR(S): Teller, Steffen; Eluwa, Stella; Koller, Markus; Uecker, Andrea; Beckers, Thomas; Baasner, Silke; Bohmer, Frank-D.; Mahboobi, Siavosh  
CORPORATE SOURCE: Research Unit Molecular Cell Biology, Medical Faculty, Friedrich Schiller University, Jena, D-07747, Germany  
SOURCE: European Journal of Medicinal Chemistry (2000), 35(4), 413-427

PUBLISHER: Editions Scientifiques et Medicales Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Members of the structurally diverse family of  $\beta$ -carbolines have previously been shown to exhibit a wide range of biol. activities. A novel synthetic strategy for generation of  $\beta$ -carbolines was developed, allowing imido- $\beta$ -carbolines to be created in three steps from known compds. The compds. were screened for inhibition of platelet-derived growth factor (PDGF)-stimulated tyrosine phosphorylation in Swiss 3T3 fibroblasts. A number of the newly synthesized  $\beta$ -carbolines with moderate to potent inhibitory activity were revealed.  $\beta$ -Carboline I was found to be the most active derivative inhibiting purified PDGF receptor kinase and PDGF-receptor autophosphorylation in intact cells with IC<sub>50</sub> values of 0.4 and 2.6  $\mu$ M, resp. I also inhibited PDGF-stimulated DNA synthesis in Swiss 3T3 fibroblasts with an IC<sub>50</sub> of 3.2  $\mu$ M. The compound had no effect on Src or epidermal growth factor (EGF) receptor kinase activity and a six-seven-fold higher IC<sub>50</sub> for inhibition of basic fibroblast growth factor (bFGF)-stimulated tyrosine phosphorylation or Kit/stem cell factor (SCF) receptor autophosphorylation, indicating a reasonable extent of kinase specificity. Thus,  $\beta$ -carbolines present a new lead of tyrosine kinase inhibitors with the capacity to selectively interfere with PDGF receptor signal transduction and PDGF-dependent cell growth.

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:242550 HCAPLUS

DOCUMENT NUMBER: 133:236049

TITLE: A refined model for monitoring orthotropic tumor growth in nude mice

AUTHOR(S): Klenner, T.; Beckers, T.; Westhof, A.; Baasner, S.; Hilgard, P.

CORPORATE SOURCE: Department of Cancer Research, ASTA Medica AG, Frankfurt/Main, Germany

SOURCE: Contributions to Oncology (1999), 54 (Relevance of Tumor Models for Anticancer Drug Development), 101-108  
 CODEN: COONEV; ISSN: 0250-3220

PUBLISHER: S. Karger AG



DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Athymic nude mice are commonly used in cancer research as hosts for xenografts of human tumors or oncogene-transformed recombinant cell lines. Tumorigenesis induced by the receptor tyrosine kinase HER2 was studied in vivo using the tTA/tetO7 system to allow conditional HER2 overexpression in NIH 3T3 fibroblasts. The tetoff system allows for a differential control of gene expression which is switched off by increasing concns. of tetracyclines. Because the expression of HER2 is related to the marker gene human secreted placental-type alkaline phosphatase (SEAP), tumor cell growth can be monitored in vitro and in vivo by simply measuring SEAP in culture supernatants or animal serum. Thus, a target-specific xenograft model was developed. However, it might be possible to use SEAP in other cell lines. Hence, the surgical methods were combined with the mol. biol. methods. SEAP was employed as a reporter gene for transfection of human tumor cell lines to develop a more sensitive, reliable and generally applicable method for monitoring tumor growth in nude mice independent of the location of the tumor.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:351174 HCAPLUS

DOCUMENT NUMBER: 126:312250

TITLE: Tumor cell lines using the human placenta-specific alkaline phosphatase gene as a reporter in the screening of antitumor-compositions

INVENTOR(S): Beckers, Thomas; Klenner, Thomas; Baasner, Silke

PATENT ASSIGNEE(S): Asta Medica Aktiengesellschaft, Germany; Zentaris GmbH; Asta Medica Oncology GmbH & Co.

SOURCE: Eur. Pat. Appl., 26 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 773293	A2	19970514	EP 1996-117448	19961030
EP 773293	A3	19981230		
EP 773293	B1	20031203		
R: CH, DE, FR, GB, LI				
DE 19542051	A1	19970515	DE 1995-19542051	19951110
DE 19542051	C2	20000323		
US 5837462	A	19981117	US 1996-746383	19961108
JP 09131184	A2	19970520	JP 1996-312624	19961111
			DE 1995-19542051	A 19951110

PRIORITY APPLN. INFO.:

AB Tumor cell lines carrying an expression cassette for the secreted human placental alkaline phosphatase (SEAP) are described for use in the screening of compds. for their effectiveness as antitumor compds. These cells can be used for implantation into a test animal or in culture. Serum levels of the enzyme are proportional to the number of cells in the animal and can be used to measure rates of tumor growth before the tumor forms a palpable mass. Dicistronic expression constructs are used. The constructs use a constitutive or inducible promoter to drive expression of a gene that can induce tumorigenic growth of cells, e.g. erb2/HER2, an IRES, and the gene for SEAP with the two genes in any order. The development of an in vivo system using the c-erbB2 gene in a dicistronic construct with the SEAP

gene is described. A constitutive expression cassette using the SV40 immediate-early promoter and an inducible cassette using a tetracycline-responsive operator are described.

L20 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:612409 HCAPLUS

DOCUMENT NUMBER: 125:272260

TITLE: Reversible tumorigenesis in mice by conditional expression of the HER2/c-erbB2 receptor tyrosine kinase .

AUTHOR(S): Baasner, Silke; von Melchner, Harald; Klenner, Thomas; Hilgard, Peter; Beckers, Thomas

CORPORATE SOURCE: Department of Cancer Research, ASTA Medica AG, Frankfurt/Main, 60314, Germany

SOURCE: Oncogene (1996), 13(5), 901-911

CODEN: ONCNES; ISSN: 0950-9232

PUBLISHER: Stockton

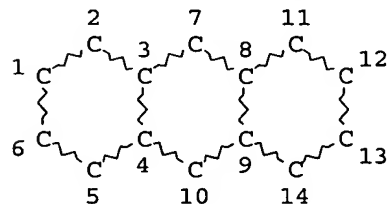
DOCUMENT TYPE: Journal

LANGUAGE: English

AB In the present study we describe the reversible transformation of NIH3T3 fibroblasts by overexpression of the HER2/c-erbB2 receptor tyrosine kinase. Cell lines expressing HER2 under control of a tetracycline-responsive promoter were isolated. Induction of HER2 expression resulted in cellular transformation in vitro as depicted by growth in soft agar and focus formation in tissue culture. Subsequent treatment of these cells with the effector anhydrotetracyclin switched-off HER2 expression and induced morphol. and functional changes characteristic for non-transformed cells. S.c. transplantation of cells in nude mice resulted in the formation of solid tumors. Interestingly tumor formation was completely suppressed by treatment of the animals with anhydrotetracycline. Our findings indicate that overexpression of HER2 induces the transformed phenotype of NIH3T3 cells and is required for tumor formation and progression in nude mice. By linking the expression of the marker gene secreted placental alkaline phosphatase to the expression of HER2, a sensitive monitoring of tumor development in nude mice was feasible.

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L5 STR



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DEFAULT ECLEVEL IS LIMITED

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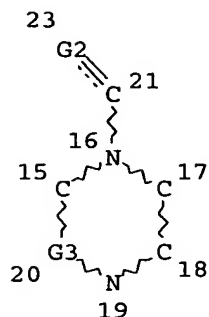
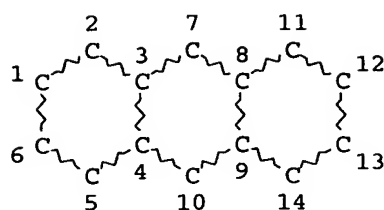
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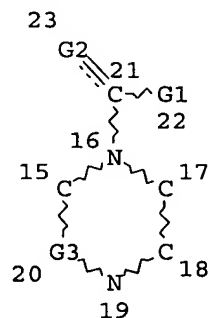
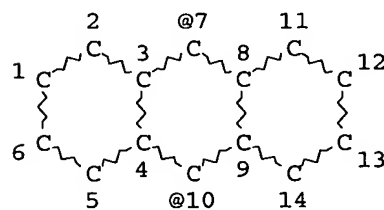
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L23 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:587287 HCAPLUS

DOCUMENT NUMBER: 131:266704

TITLE: Anticancer drug sensitivity and expression of multidrug resistance markers in early passage human sarcomas

AUTHOR(S): Hoffmann, Jens; Schmidt-Peter, Peter; Hansch, Wolfgang; Naundorf, Helga; Bunge, Andreas; Becker, Michael; Fichtner, Iduna

CORPORATE SOURCE: Max-Delbrück-Center of Molecular Medicine, Berlin, 13122, Germany

SOURCE: Clinical Cancer Research (1999), 5(8), 2198-2204  
CODEN: CCREF4; ISSN: 1078-0432

PUBLISHER: American Association for Cancer Research

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We have established new human sarcoma lines and examined their sensitivity to common antitumor drugs and expression of putative multidrug resistance (MDR) proteins. Eighty-two sarcoma samples were transplanted in nude mice. Fourteen of these sarcomas were established as tumor cell lines. We determined a chemosensitivity profile to antitumor drugs (MDR drugs = doxorubicin, mitoxantrone, and vincristine; non-MDR drugs = cisplatin, ifosfamide, and bleomycin) for each tumor line in vivo. Response to chemotherapy with doxorubicin and ifosfamide was observed in 30-50% of these tumor lines. Our results obtained with xenotransplants are similar to the results documented in clin. trials in which doxorubicin and ifosfamide are effective in 30-50% of the patients. Furthermore, we examined expression of MDR-relevant markers like P-glycoprotein, MDR-associated protein, lung resistance protein, and mdrl mRNA in these xenotransplants. A relationship between mdrl mRNA expression and response to doxorubicin was demonstrated in >90% of our tumor lines. In six sarcomas with mdrl mRNA expression, five were resistant against doxorubicin and cross-resistant

against several other drugs, whereas from eight sarcomas, which lacked detectable *mdr1* mRNA, seven were sensitive to doxorubicin and other drugs. We found lung resistance protein or MDR-associated protein expressed in three resistant and *mdr1* mRNA-pos. sarcomas. These results demonstrate that *mdr1* mRNA expression is a putative marker for drug resistance in our sarcoma lines. We conclude, therefore, that inherent P-glycoprotein expression might be also responsible for drug resistance occurring in treatment of patients with sarcomas. The established tumor lines are useful for addnl. investigations on mechanisms of drug resistance in sarcomas and as models for preclin. screening of new antitumor drugs.

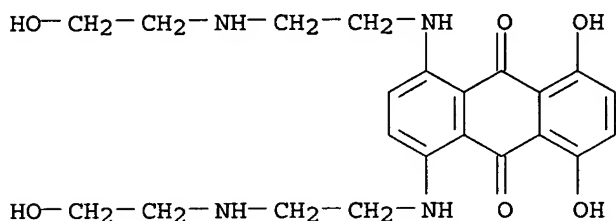
IT 65271-80-9, Mitoxantrone

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(anticancer drug sensitivity and expression of multidrug resistance markers in early passage human sarcomas)

RN 65271-80-9 HCAPLUS

CN 9,10-Anthracenedione, 1,4-dihydroxy-5,8-bis[[2-[(2-hydroxyethyl)amino]ethyl]amino]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:618071 HCAPLUS

DOCUMENT NUMBER: 113:218071

TITLE: Development of a suspension-emulsion system for parenteral application in animals

AUTHOR(S): Schmidt, Peter C.; Perschbacher, Harald; Steffens, Klaus Juergen; Kraemer, Hans P.

CORPORATE SOURCE: Dep. Pharm. Technol., Univ. Tuebingen, Tuebingen, Fed. Rep. Ger.

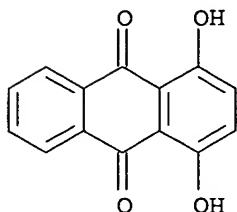
SOURCE: Acta Pharmaceutica Technologica (1989), 35(1), 34-7  
CODEN: APTEDD; ISSN: 0340-3157

DOCUMENT TYPE: Journal

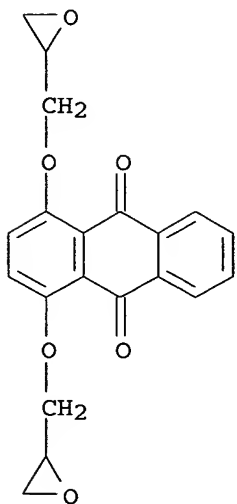
LANGUAGE: English

AB The pharmacol. activities of a new suspension-emulsion formulation of 2 antineoplastic drugs and spironolactone, all 3 only very slightly soluble in water and oils, were tested in mice and rats. The active ingredients were ground in medium chain triglycerides using a wet ball milling process. The resulting suspension was incorporated in an oil-water emulsion using lecithin and cholesterol as emulsifiers and then homogenized by a high-pressure homogenization process. The particle size of this suspension-emulsion system was in the range of 1 to 2  $\mu\text{m}$  with a few particles up to 7  $\mu\text{m}$ . In vivo results showed an increased bioavailability of the antineoplastic drugs when compared with an aqueous suspension. Spironolactone was more effective after i.p. administration than after i.v. application, but did not reach the effect of K canrenoate. The formulations were all well tolerated by the animals.

IT 81-64-1, 1,4-Dihydroxyanthraquinone 98298-55-6, S 830544  
 RL: BIOL (Biological study)  
 (suspension-emulsion parenteral system containing, development and  
 bioavailability of)  
 RN 81-64-1 HCAPLUS  
 CN 9,10-Anthracenedione, 1,4-dihydroxy- (9CI) (CA INDEX NAME)



RN 98298-55-6 HCAPLUS  
 CN 9,10-Anthracenedione, 1,4-bis(oxiranylmethoxy)- (9CI) (CA INDEX NAME)



L23 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1989:445270 HCAPLUS  
 DOCUMENT NUMBER: 111:45270  
 TITLE: Pharmaceutical emulsions containing an oily phase,  
 lecithin, an electrolyte and solid active agents  
 INVENTOR(S): List, Paul Heinz; Schmidt, Peter Christian;  
 Steffens, Klaus Juergen; Perschbacher, Harald;  
 Kraemer, Hans Peter; Sedlacek, Hans Harald  
 PATENT ASSIGNEE(S): Behringwerke A.-G., Fed. Rep. Ger.  
 SOURCE: Ger. Offen., 6 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DE 3623376	A1	19880121	DE 1986-3623376	19860711
EP 256285	A1	19880224	EP 1987-109765	19870707
EP 256285	B1	19910320		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AT 61730	E	19910415	AT 1987-109765	19870707
ES 2039214	T3	19930916	ES 1987-109765	19870707
FI 8703044	A	19880112	FI 1987-3044	19870709
US 4801455	A	19890131	US 1987-71382	19870709
DK 8703597	A	19880112	DK 1987-3597	19870710
AU 8775536	A1	19880114	AU 1987-75536	19870710
AU 597688	B2	19900607		
JP 63023811	A2	19880201	JP 1987-171323	19870710
ZA 8705044	A	19880224	ZA 1987-5044	19870710
CA 1302257	A1	19920602	CA 1987-541803	19870710

## PRIORITY APPLN. INFO.:

DE 1986-3623376	A	19860711
EP 1987-109765	A	19870707

AB The title composition is suitable for the parenteral formulation of difficult to solubilize active agents; it contains a solid/liquid/liquid disperse system with particle size  $\leq 5 \mu\text{m}$  which is obtained by emulsifying a ground substance with particle size  $\leq 3 \mu\text{m}$  1.5, an oily phase 8-30, an emulsifier 1.0-45, and H<sub>2</sub>O 64-90% by weight. This emulsion is adjusted to isotonic conditions and homogenized in a high-pressure homogenizer. A 10% suspension of danthron (I) in Miglyol 812 (II) was ground to a particle size  $< 3 \mu\text{m}$ ; this was diluted 1-fold with II, and then was diluted with 24% lecithin in II, and this was mixed with cholesterol, H<sub>2</sub>O, and finally with NaCl, and finally homogenized. The product (40 g) contained I 0.200, II 3.800, Epikuron 170 (lecithin) 0.480, cholesterol 0.048, and 0.9% NaCl 35.472 g. A formulation (40 g) containing S830544 (anthraquinone derivative) 0.0124, II 3.9876, Epikuron 170 0.48, cholesterol 0.048, and NaCl 35.472 g was administered daily (4.64 mg/kg) to mice inoculated with 106 L1210 leukemia cells; the ratio of median survival time vs. an untreated control (MT/C) was 125%, whereas for mice treated with S830544 (200 mg/kg) in a tenside-containing medium the MT/C was 100%.

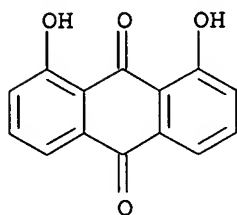
IT 117-10-2 98298-55-6, S 830544

RL: BIOL (Biological study)

(pharmaceutical parenteral emulsion containing)

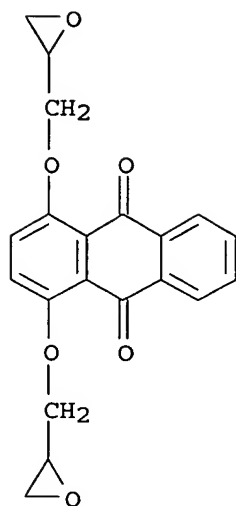
RN 117-10-2 HCAPLUS

CN 9,10-Anthracenedione, 1,8-dihydroxy- (9CI) (CA INDEX NAME)



RN 98298-55-6 HCAPLUS

CN 9,10-Anthracenedione, 1,4-bis(oxiranylmethoxy)- (9CI) (CA INDEX NAME)



L23 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:534786 HCAPLUS

DOCUMENT NUMBER: 107:134786

TITLE: The action of anthraquinone sensitizers in the photo-oxidative degradation of low density polyethylene: mechanical evidence of dark processes

AUTHOR(S): Raab, M.; Hnat, V.; Schmidt, P.; Kotulak, L.; Taimr, L.; Pospisil, J.

CORPORATE SOURCE: Inst. Macromol. Chem., Czech. Acad. Sci., Prague, 162 06, Czech.

SOURCE: Polymer Degradation and Stability (1987), 18(2), 123-34

CODEN: PDSTDW; ISSN: 0141-3910

DOCUMENT TYPE: Journal

LANGUAGE: English

AB LDPE films containing 3 quinoid sensitizers, anthraquinone (I), 2-butylanthraquinone (II), and 2-octanoyloxyanthraquinone (III), were exposed to the UV light of a fluorescent tube. The kinetics of the photooxidative degradation was monitored by measuring IR spectra and 3 mech. characteristics derived from stress-strain traces, viz. strain at break, Young's modulus, and yield stress. During the first stage of the process, the greater solubility of II and III in LDPE compared to I was clearly manifested in both the mech. and spectral data. The sensitizers were consumed at the very beginning of the exposure, but once the degradation started it continued at a higher rate around introduced or intrinsic centers. The increase of yield stress values after a long-term dark storage which followed the irradiation period was ascribed to a slow continuous crystallization of the degraded polymer. No dark storage effect was found with samples not previously exposed to UV light.

IT 84-65-1, Anthraquinone 7504-51-0, 2-Butylanthraquinone 110484-84-9

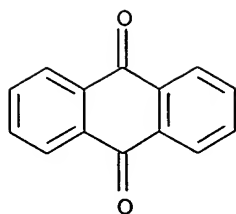
RL: USES (Uses)

(sensitizers, in photooxidative degradation of LDPE)

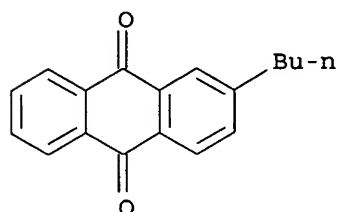
RN 84-65-1 HCAPLUS

CN 9,10-Anthracenedione (9CI) (CA INDEX NAME)

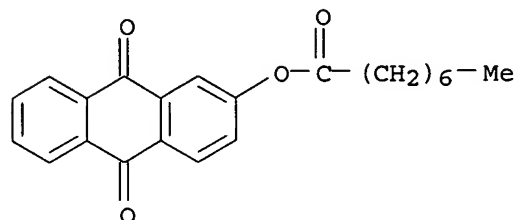




RN 7504-51-0 HCAPLUS  
CN 9,10-Anthracenedione, 2-butyl- (9CI) (CA INDEX NAME)



RN 110484-84-9 HCAPLUS  
CN Octanoic acid, 9,10-dihydro-9,10-dioxo-2-anthracenyl ester (9CI) (CA INDEX NAME)



L23 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1984:111413 HCAPLUS  
DOCUMENT NUMBER: 100:111413  
TITLE: Optical absorption of molecules in the electric field of the double layer  
AUTHOR(S): Schmidt, P.; Plieth, W.  
CORPORATE SOURCE: Inst. Phys. Chem., Freie Univ., Berlin, D-1000/33, Fed. Rep. Ger.  
SOURCE: Journal de Physique, Colloque (1983), (C10), 175-8  
CODEN: JPQCAK; ISSN: 0449-1947  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The structures and properties of organic monolayers adsorbed on a polished Pt electrode were studied with the help of modulation reflectance (MR) spectroscopy. The monolayers of p-aminonitrobenzene, p-(dimethylamino)nitrosobenzene, and p-(dimethylamino)nitrostilbene show electrochromic effects which allow the determination of the orientation of the adsorbed mols. and finally the calcn. of the double layer field strength. In addition to that, the MR spectrum of anthracene adsorbed on a Pt electrode

was also detected.

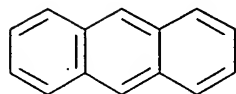
IT 120-12-7, properties

RL: PRP (Properties)

(modulated reflectance spectra of, adsorbed on platinum electrode)

RN 120-12-7 HCAPLUS

CN Anthracene (8CI, 9CI) (CA INDEX NAME)



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